

Advanced Scientific Computing Research

Program Mission

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. This scientific leadership is critical to the economic health of the nation. The mission of the Advanced Scientific Computing Research (ASCR) program is to underpin DOE's world leadership in scientific computation by supporting research in applied mathematics, computer science and high-performance networks and providing the high-performance computational and networking resources that are required for world leadership in science.

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 research programs in the U.S. Department of Energy's Office of Science—in Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, and High Energy 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 the Office of Science. 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. In March 2002, Japan's NEC Earth Simulator became operational. With a peak speed of 40 teraflops and a demonstrated sustained capability of over 25 teraflops, it is faster by approximately a factor of 50 than the most advanced supercomputer for civilian science in the United States. The potential long-term implications of the Earth Simulator on DOE's computational sciences capability was the principal message of the report on this subject delivered to the Director of the Office of Science by the Advanced Scientific Computing Advisory Committee. To strengthen the program's position in this area, the ASCR program is proposing a new effort in Next Generation Computer Architecture (NGA) to identify and address major bottlenecks in the performance of existing and planned DOE science applications.

The ASCR program supports the Office of Science Strategic Plan's goal of providing extraordinary tools for extraordinary science as well as building the foundation for the research in support of the other goals of the strategic plan. The research programs of ASCR have played a critical role in the evolution of high performance computing and networks. The ASCR program actively contributes to the goals of the *Five Year Strategic Plan* of the Interagency Working Group on Information Technology R&D. In particular, ASCR plays a key role in Large Scale Networking and High End Computing and Computation.

The ASCR program is also responsible for the Laboratory Technology Research subprogram, whose mission is to foster and support high-risk research in the natural sciences and engineering in partnership with the private sector leading to innovative applications relevant to the Nation's energy sector.

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.

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.

Advisory and Consultative Activities:

The *Advanced Scientific Computing Advisory Committee (ASCAC)*, established on August 12, 1999, provides valuable, independent advice to the Department of Energy 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 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 Director, Office of Science 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; 92nd Congress, H.R. 4383; October 6, 1972) 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 ITWG evolved through an interagency coordination process that began under the 1991 High Performance Computing Act as the High Performance Computing, Communications, and Information Technology (HPC/CIT) Committee. The Federal IT R&D agencies have established a 10-year record 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 National Science and Technology Council and the President's Science Advisor.

ASCR is a participant in the Interagency Committee for Extramural Mathematics Programs (ICEMAP), a coordinating committee with representatives from federal agencies that manage programs in mathematical research, including the National Science Foundation, DOE (through ASCR), the National Aeronautics and Space Administration, the National Institute for Standards and Technology, the Air Force Office of Scientific Research, the Army Research Office, and the Office of Naval Research. Meetings are held to coordinate activities across mathematical research programs, ensuring that the federal agencies coordinate their investments in basic mathematical research. The ASCR program regards ICEMAP as an important component in their efforts to maintain coordination with other federal agencies.

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), and the Advanced Computing Research Testbeds (ACRTs).

NERSC, operated by the Lawrence Berkeley National Laboratory, annually serves about 2,400 scientists throughout the United States. 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 Office of Science goals and objectives and the readiness of the proposed application to fully utilize the computing resources being requested.

The ESnet, managed and operated by the Lawrence Berkeley National Laboratory, is a high-speed network serving thousands of Department of Energy scientists and collaborators worldwide. A pioneer in providing high-bandwidth, reliable connections, ESnet enables researchers at national laboratories, universities and other institutions to communicate with each other using the collaborative capabilities 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 the Office of Science programs. All program offices in the Office of Science appoint members, who represent their scientific communities, 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 external peer reviews of ESnet performance on a three year interval. The last such review was chaired by a member of ASCAC and took place in September 2001.

Advanced Computing Research Testbeds (ACRTs) play a critical role in testing and evaluating new computing hardware and software. Current testbeds are located at Oak Ridge National Laboratory (IBM Power-4 Technology and CRAY X1 technology). In FY 2002, ASCAC conducted a review of the NERSC and ACRTs. 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 Office of Science over the next three to five years?

The essential finding of the Subcommittee is that NERSC and the ACRTs are among the best worldwide in their respective categories. It is the opinion of the Subcommittee that these ASCR activities and the

related spin-off research efforts contribute significantly to the mission needs of the DOE, and profoundly and positively impact high performance computing activities worldwide. The complete report is available on the web at: <http://www.sc.doe.gov/ascr/ASCAC-sub.doc>

In FY 2001, ASCR conducted a peer review of the Center for Computational Sciences (CCS) at the Oak Ridge National Laboratory. The findings from this review validated the contributions that the CCS made to the Advanced Computing Research Testbed activity within the ASCR program.

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 2002, ASCAC conducted a review of NERSC and the ACRTs.

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 percent of this activity. In FY 2004, ASCR will conduct 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 percent of this activity. In FY 2005, ASCR will conduct a peer review of the remaining 34 percent of the Applied Mathematics activity, which consists of Computational Fluid Dynamics and Meshing Techniques. In FY 2004, ASCR will initiate a comprehensive review of the Computer Science research activity.

In FY 2002, following a comprehensive peer review, the ASCR program approved a proposal from the Lawrence Berkeley National Laboratory (LBNL) to manage and operate the National Energy Research Scientific Computing Center for FY 2002 – FY 2006.

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 advance 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:

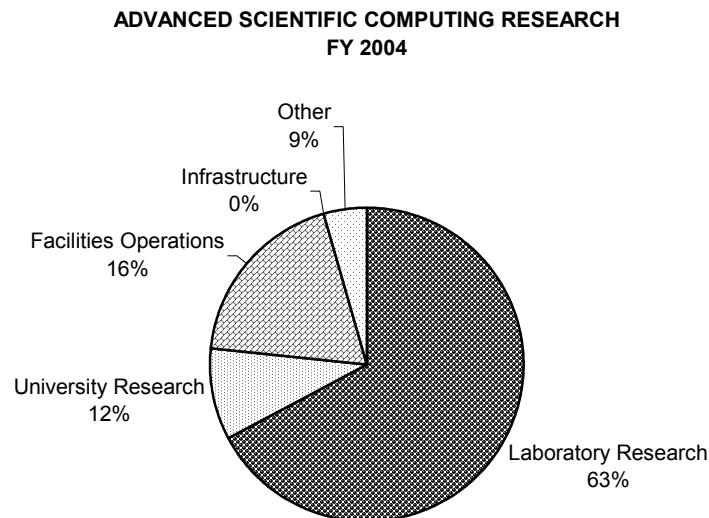
- The Department and Office of Science Strategic Plan, as updated through program collaborations and joint advisory committee meetings. http://www.science.doe.gov/production/bes/strat_pln.htm
- Scientific Discovery through Advanced Computing (SciDAC) plan delivered to Congress in March 2000. <http://www.science.doe.gov/scidac/>
- The Interagency Working group for Information Technology Five Year Plan – FY 2002-FY 2006 (with key appendixes)
- ASCAC report on the Japanese Earth Simulator. <http://www.sc.doe.gov/ascr/ascac.reports.htm>

How We Spend Our Budget:

The ASCR program budget has two major components: research and facility testbed and network operations. The FY 2004 budget request continues the core and SciDAC research efforts and strengthens the research partnerships with other SC offices. The testbed and network operations expenditures account for 37 percent of the National Lab Research, or 24 percent of the total ASCR budget.

Research:

Over 76 percent of the program's FY 2004 funding will be provided to scientists at universities and laboratories to conceive and carry out the research or to fund advanced computing testbeds and network operations. National laboratory research scientists work together with the other programs of the Office of Science 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 2002, 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. These grants included support for graduate students. In addition, ASCR supports a Computational Science Graduate Fellowship and an Early Career Principal Investigator Program in Applied Mathematics, Computer Science and High-Performance Networks. In FY 2002, ASCR selected 24 new graduate fellows representing 17 universities and 13 states and expects to make up to forty awards to early career principal investigators. ASCR also provides support to other Office of Science research programs. Approximately one-half of those who received Ph.D.'s in the Computational Sciences Graduate Fellowship program between 1991 and 2001 are pursuing careers outside universities or national labs.

The university grants program is proposal driven, similar to the computer science and applied mathematics programs at 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 (see: www.er.doe.gov/production/grants/grants.html). Proposals are reviewed by external scientific peers and competitively awarded according to the guidelines published in 10 CFR 605 (www.science.doe.gov/production/grants/605index.html).

- National Laboratory Research:** ASCR supports national laboratory-based research groups at Ames, Argonne, Brookhaven, Los Alamos, Lawrence Berkeley, Lawrence Livermore, Oak Ridge, Pacific Northwest, and Sandia National Laboratories. 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 the Office of Science. Laboratory researchers collaborate with laboratory and academic researchers, and are important for developing and maintaining testbeds and novel applications of high performance computing and networking in Office of Science research. At Los Alamos, Livermore and Sandia, ASCR funding plays an important role in supporting basic research that can improve the applied programs, such as the Accelerated Strategic Computing Initiative (ASCI) and the Science Stockpile Stewardship program.

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.

Program Strategic Performance Goals

- SC5-1:** Build leading research programs in focused disciplines of applied mathematics, computer science, and network and collaborative research important to national and energy security to spur revolutionary advances in the use of high performance computers and networks. (Mathematical, Information and Computational Sciences subprogram)

Performance Indicator

Eighty percent of all new research projects will be peer reviewed and deemed excellent and relevant, and annually 30 percent of all ongoing projects will be subject to peer review with merit evaluation; all research areas and facilities will be periodically reviewed by subcommittees of the Advanced Scientific Computing Advisory Committee and determined to be world class.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Completed the development of the Cougar lightweight kernel for clusters of Alpha processor-based computers and begin the assessment of scalability and performance for selected applications. (SC5-1) [Met Goal]	Complete the definitive analysis of the advantages and issues associated with lightweight kernel operating systems rather than full kernels for the compute nodes of extreme-scale scientific computers, resolving a critical issue for the future of high performance computers in the U.S. (SC5-1)	Define, based on the analysis completed in FY 2003, a research strategy that will deliver by 2007 effective operating systems for high performance scientific computers with 20,000 or more processors. (SC5-1) Complete, by the end of FY 2004, a roadmap that defines the critical, applied mathematics research issues which must be addressed to enable the development of mathematical algorithms that can operate efficiently on computers with thousands of

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
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Appointed 25 new students to the Computational Science Graduate Fellowship Program to develop the next generation of leaders in computational science for DOE and the Nation. (SC5-1) [Exceeded Goal]

processors and address the needs of DOE mission applications. This roadmap will be completed through a series of workshops sponsored by ASCR and ASCAC.

Respond to recommendations of Advanced Scientific Computing Advisory Committee sub panel on computational biology.

SC5-2: Create the Mathematical and Computing Systems Software and the High Performance Computing Facilities that enable Scientific Simulation and Modeling Codes to take full advantage of the extraordinary capabilities of terascale (trillions of operations per second) computers, and the Collaboratory Software Infrastructure to enable geographically-separated scientists to effectively work together as a team as well as provide electronic access to both facilities and data. (Mathematical, Information and Computational Sciences subprogram)

Performance Indicator

Validation of results by merit review with external peer evaluation.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
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Achieved operation of the IBM-SP computer at 5.0 Teraflop “peak” performance. These computational resources will be integrated by a common high performance file storage system that facilitates interdisciplinary collaborations. (SC5-2) [Met Goal]

Begin installation of next generation NERSC computer, NERSC-4, that will at least double the capability available in FY 2002 to solve leading edge scientific problems. (SC5-2)

Complete installation of next generation NERSC computer, NERSC-3e, that will at least double the capability available to solve leading edge scientific problems. The number of Massively Parallel Processor Hours (MPP Hours) available will increase from 53 million in FY 2003 to 110 million in FY 2004.

Migrated the users with the largest allocations to the IBM-SP from the previous generation Cray T3E. (SC5-2) [Met Goal]

Initiate at least 8 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

Deliver enhanced versions of software from Integrated Software Infrastructure Centers established in FY 2001 to scientific application research teams. This software will increase the average efficiency of those applications by 50% (from the current 10% average baseline efficiency of peak processor power to 15%). This improvement in efficiency

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
	Biological and Environmental Research and Basic Energy Sciences programs, respectively, of submitted proposals. (SC5-2)	will enable a 30% increase in the amount of science research/analysis that can be accomplished at the existing high performance computing facilities.
	Evaluate effectiveness of a new software tool-(GRID middleware) as a tool to enable SC user communities in High Energy Physics and Global Climate to effectively access very large data resources over the Internet.	Plan upgrade of ESnet that will satisfy transatlantic data requirements of Large Hadron Collider (LHC) experiment at CERN outside of Geneva, Switzerland.

SC7-5: Provide advanced scientific user facilities where scientific excellence is validated by external review; average operational downtime does not exceed 10 percent of schedule; construction and upgrades are within 10 percent of schedule and budget; and facility technology research and development programs meet their goals. (Mathematical, Information and Computational Sciences subprogram)

Performance Indicator

Percent unscheduled downtime.

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Targets	FY 2004 Targets
Maintained and operated facilities, including NERSC and ESnet, so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time.[Met Goal]	Maintain and operate facilities, including NERSC and ESnet, so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. (SC7-5)	Maintain and operate facilities, including NERSC and ESnet, so the unscheduled downtime on average is less than 10 percent of the total scheduled operating time. (SC7-5)
Deliver preliminary report of ASCAC review of ASCR high performance computing facilities. (SC7-5) [Met Goal]	Complete the review of ASCR high performance computing facilities by the Advanced Scientific Computing Advisory Committee (ASCAC) and implement action plans to respond to recommendations. (SC7-5)	Complete the review of ASCR high performance network facilities by the Advanced Scientific Computing Advisory Committee (ASCAC) and implement action plans to respond to recommendations.

Program Assessment Rating Tool (PART) Assessment

The Office of Management and Budget has provided the ASCR program with input using their Program Assessment Rating Tool (PART). The OMB states that ASCR's program has a fairly well defined mission and merit-based reviews for awarding contracts and grants, leading to high scores for both purpose and management practices. Despite the problems inherent in predicting and then measuring scientific progress, the OMB has acknowledged that ASCR has made significant strides in developing long-term and annual performance measures. The OMB also stated that in the past several years, ASCR has recast its focus between several large initiatives since 2000. The OMB suggested that this situation reflected a lack of long-term vision for the program, and recommended that ASCR develop a long-term strategic plan. The OMB also noted that the ASCR program does not yet have regular reviews of its research portfolio and processes by a Committee of Visitors (COV). Both suggestions have been adopted by ASCR as action items to be completed by the end of FY 2003.

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.

High-performance computing and networking resources will be provided to meet the needs of the base research programs throughout the Office of Science. Research efforts initiated in FY 2001 in Scientific Discovery through Advanced Computing (SciDAC) will be continued, as planned. The FY 2004 budget includes \$13,968,000 to launch a research investment in Next Generation Computer Architecture for science. The NGA will increase the delivered computing capability available to address the Office of Science mission through optimization of computer architectures to meet the special requirements of scientific problems. This investment positions the nation to realize extraordinary scientific opportunities in computing for science and enable new classes of scientific problems to be addressed. The NGA effort complements SciDAC and integrates advanced computer architecture researchers and engineers, application scientists, computer scientists, and applied mathematicians.

The computational needs of the SciDAC research program will be addressed by investments focused on providing high-performance computing pilot capability for Topical Applications. The FY 2004 budget request includes \$7,867,000 for continued support of the Genomes to Life research program, in partnership with the Biological and Environmental Research program; and \$3,072,000 for the Nanoscale Science, Engineering and Technology initiative led by the Basic Energy Sciences program. ASCR's contributions to these partnerships will consist of advancing the mathematics and developing new mathematical algorithms to simulate biological systems and physical systems at the nanoscale.

In FY 2004, the Mathematical, Information and Computational Sciences subprogram will continue to support core research activities at current levels.

The Laboratory Technology Research subprogram will be brought to a successful conclusion in FY 2004.

Interagency Environment

The activities funded by the MICS subprogram 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 ITWG 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. 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 2004 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: acting as a technical agent for one of the DARPA High Productivity Computing Systems contracts; serving on the planning group for the Congressionally mandated DOD plan for high performance computing to serve the national security mission; and extensive collaboration with NNSA-Advanced Simulation Computing.

Scientific Discovery through Advanced Computing

The SciDAC activity is a set of coordinated investments across all Office of Science mission areas with the goal to achieve breakthrough scientific advances through computer simulation that were impossible using theoretical or laboratory studies alone. By exploiting advances in computing and information technologies as tools for discovery, SciDAC encourages and enables a new model for multi-discipline collaboration among the scientific disciplines, computer scientists and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can fully exploit terascale computing and networking resources. The program will bring simulation to a parity level with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate prediction, plasma physics, particle physics, astrophysics and computational chemistry.

Next Generation Computer Architecture

The goal of the Next Generation Computer Architecture (NGA) research activity is to identify and address major architectural bottlenecks, such as internal data movement in very large systems, in the performance of existing and planned DOE science applications. Emphasis will be placed on understanding the impact of alternative computer architectures on application performance with particular attention paid to data movement from memory to processor and between processors in highly parallel systems. Software research will be initiated to improve application performance and system reliability through innovative approaches to next generation operating systems. Emphasis will also be placed on hardware evaluation testbeds of sufficient size to understand key issues impacting application performance scalability and portability. The NGA activity will be coordinated with other Federal agencies to gain additional insight into research directions, optimize the utilization of resources, and establish the framework for a national effort.

Scientific Facilities Utilization

The ASCR program request includes support to the National Energy Research Scientific Computing (NERSC) Center, a component of the Office of Science-wide Scientific Facilities Initiative. This investment will provide computer resources for about 2,400 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 Office of Science research programs.

(hours)	FY 2000	FY 2001	FY 2002	FY 2003 Est.	FY 2004 Est.
Maximum Hours – NERSC	8,760	8,760	8,760	8,760	8,760
Scheduled Hours – NERSC	8,497	8,585	8,585	8,585	8,585
Unscheduled Downtime – NERSC	1%	1%	1%	–	–

Workforce Development

The R&D Workforce Development mission is to ensure the supply of computational and computer science and Ph.D. level scientists for the Department and the Nation through graduate student and postdoctoral research support. In FY 2004, this program will support approximately 800 graduate students and post doctoral investigators, of which 500 will be supported at Office of Science user facilities.

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

	FY 2000	FY 2001	FY 2002	FY 2003 est.	FY 2004 est.
# University Grants	128	170	163	144	140
Size, Duration	\$95,000/yr- 3 yrs	\$157,000/yr- 3yrs	\$157,000/yr- 3yrs	\$197,000/yr- 3yrs	\$197,000/yr- 3yrs
# Lab Groups	148	226	209	165	165
# Grad Students	290	370	354	354	354
# PhD's Awarded	550	660	604	675	675

Funding Profile

(dollars in thousands)

	FY 2002 Comparable Appropriation	FY 2003 Request	FY 2004 Request	\$ Change	% Change
Advanced Scientific Computing Research					
Mathematical, Information, and Computational Sciences.....	147,159	163,557	170,490	+6,933	+4.2%
Laboratory Technology Research.....	3,046	3,000	3,000	0	--
Total, Advanced Scientific Computing Research.....	150,205^{abc}	166,557^c	173,490	+6,933	+4.2%

Public Law Authorization:

Public Law 95-91, "Department of Energy Organization Act"

Public Law 103-62, "Government Performance and Results Act of 1993"

^a Excludes \$3,731,000 which was transferred to the SBIR program and \$224,000 which was transferred to the STTR program.

^b Excludes \$88,000 for the FY 20023 rescission contained in section 1403 of P.L. 107-226, Supplemental Appropriations for further recovery from and response to Terrorist attacks on the United States.

^c Excludes \$3,068,000 in FY 2002, FY 2003 and FY 2004 for Homeland Security activities that are funded in a separate Department of Homeland Security budget.

Funding by Site^a

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	\$ Change	% Change
Albuquerque Operations Office					
Los Alamos National Laboratory.....	3,709	5,020	3,570	-1,450	-28.9%
Sandia National Laboratories	5,783	3,889	6,047	+2,158	+55.5%
Total, Albuquerque Operations Office.....	9,492	8,909	9,617	+708	+7.9%
Chicago Operations Office					
Ames Laboratory	2,183	1,625	1,578	-47	-2.9%
Argonne National Laboratory.....	13,503	8,573	11,646	+3,073	+35.8%
Brookhaven National Laboratory	1,359	542	960	+418	+77.1%
Fermi National Accelerator Laboratory	326	60	226	+166	+276.7%
Princeton Plasma Physics Laboratory.....	400	0	420	+420	+100.0%
Chicago Operations Office.....	17,147	7,240	24,556	+17,316	+239.2%
Total, Chicago Operations Office.....	34,918	18,040	39,386	+21,346	+118.3%
Oakland Operations Office					
Lawrence Berkeley National Laboratory.....	65,872	53,223	57,686	+4,463	+8.4%
Lawrence Livermore National Laboratory.....	4,119	0	3,068	+3,068	+100.0%
Stanford Linear Accelerator Center	702	234	613	+379	+162.0%
Oakland Operations Office	2,122	960	3,115	+2,155	+224.5%
Total, Oakland Operations Office.....	72,815	54,417	64,482	+10,065	+18.5%
Oak Ridge Operations Office					
Oak Ridge Inst. For Science and Education....	306	99	200	+101	+102.0%
Oak Ridge National Laboratory	26,629	10,496	9,819	-677	-6.4%
Thomas Jefferson National Accelerator Facility	100	0	0	0	--
Total, Oak Ridge Operations Office	27,035	10,595	10,019	-576	-5.4%
Richland Operations Office					
Pacific Northwest National Laboratory	4,097	1,003	3,601	+2,598	+259.0%
Washington Headquarters	1,848	73,593	46,385	-27,208	-37.0%
Total, Advanced Scientific Computing Research..	150,205	166,557	173,490	+6,933	+4.2%

^a On December 20, 2002, the National Nuclear Security Administration (NNSA) disestablished the Albuquerque, Oakland, and Nevada Operations Offices, renamed existing area offices as site offices, established a new Nevada Site Office, and established a single NNSA Service Center to be located in Albuquerque. Other aspects of the NNSA organizational changes will be phased in and consolidation of the Service Center in Albuquerque will be completed by September 30, 2004. For budget display purposes, DOE is displaying non-NNSA budgets by site in the traditional pre-NNSA organizational format.

Site Description

Ames Laboratory

Ames Laboratory is a Multiprogram Laboratory located on 10 acres in Ames, Iowa. The MICS subprogram at Ames Laboratory conducts research in computer science and participates on one of the SciDAC teams. The LTR subprogram at Ames conducts research in the physical, chemical, materials, mathematical, engineering, and environmental sciences through cost-shared collaborations with industry.

Argonne National Laboratory

Argonne National Laboratory (ANL) in Argonne, Illinois, is a Multiprogram Laboratory located on a 1,700 acre site in suburban Chicago. ANL has a satellite site located in Idaho Falls, Idaho. The MICS subprogram at ANL conducts basic research in mathematics and computer science, as well as research in advanced computing software tools and collaboratory tools. ANL also participates in several scientific application and collaboratory pilot projects as well as supporting an advanced computing research testbed and participates on a number of the SciDAC teams. The ANL also focuses on testing and evaluating leading edge research computers. The LTR subprogram at ANL conducts research motivated by practical energy payoffs through cost-shared collaborations with industry. The areas emphasized in the research portfolio are chemistry of ceramic membranes, separations technology, near-frictionless carbon coatings, and advanced methods for magnesium production.

Brookhaven National Laboratory

Brookhaven National Laboratory (BNL) is a Multiprogram Laboratory located on a 5,200 acre site in Upton, New York. BNL has a computing capability for Quantum Chromodynamics (QCD) simulations. The MICS subprogram at BNL participates on one of the SciDAC teams. The LTR subprogram at BNL conducts research motivated by practical energy payoffs through cost-shared collaborations with industry. The areas emphasized in the research portfolio are materials for rechargeable lithium batteries, sensors for portable data collection, catalytic production of organic chemicals, and DNA damage responses in human cells.

Fermi National Accelerator Laboratory (Fermilab)

Fermilab is located on a 6,800-acre site about 35 miles west of Chicago, Illinois. The LTR subprogram at Fermilab conducts research in areas such as superconducting magnet research, design and development, detector development and high-performance computing through cost-shared collaborations with industry.

Lawrence Berkeley National Laboratory

Lawrence Berkeley National Laboratory (LBNL) is a Multiprogram Laboratory located in Berkeley, California. The Laboratory is on a 200 acre site adjacent to the Berkeley campus of the University of California. The MICS subprogram at LBNL conducts basic research in the mathematics and computer science, as well as research in advanced computing software tools and collaboratory tools. LBNL participates in several scientific application and collaboratory pilot projects and participates on a number of the SciDAC teams. LBNL manages the Energy Sciences Network (ESnet). ESnet is one of the world's most effective and progressive science-related computer networks that provides worldwide access and communications to Office of Science (SC) facilities. In 1996, the National Energy Research Scientific Computing Center (NERSC) was moved from the Lawrence Livermore National Laboratory to LBNL. NERSC provides a range of high-performance, state-of-the-art computing resources that are a

critical element in the success of many SC research programs. The LTR subprogram at LBNL conducts research motivated by practical energy payoffs through cost-shared collaborations with industry. The areas emphasized in the research portfolio are molecular lubricants for computers, advanced material deposition systems, screening novel anti-cancer compounds, and innovative membranes for oxygen separation.

Lawrence Livermore National Laboratory

Lawrence Livermore National Laboratory (LLNL) is a Multiprogram Laboratory located on an 821 acre site in Livermore, California. The MICS subprogram at LLNL involves participation in base research and SciDAC efforts.

Los Alamos National Laboratory

Los Alamos National Laboratory (LANL) is a Multiprogram Laboratory located on a 27,000 acre site in Los Alamos, New Mexico. The Mathematical Information and Computational Sciences (MICS) subprogram at LANL conducts basic research in the mathematics and computer science and in advanced computing software tools. LANL also participates in several scientific application and collaborative pilot projects and participates on a number of the SciDAC teams.

Oak Ridge Institute for Science and Education

Oak Ridge Institute for Science and Education (ORISE) is located on 150 acres in Oak Ridge, Tennessee. ORISE provides support for education activities funded within the ASCR program.

Oak Ridge National Laboratory

Oak Ridge National Laboratory (ORNL) is a Multiprogram Laboratory located on a 24,000 acre site in Oak Ridge, Tennessee. The MICS subprogram at ORNL conducts basic research in the mathematics and computer science, as well as research in advanced computing software tools and collaborative tools. ORNL also participates in several scientific application and collaborative pilot projects and participates on a number of the SciDAC teams. ORNL also supports Advanced Computing Research Testbeds (ACRTs) focused on the evaluation of leading edge research computers. The LTR subprogram at ORNL conducts research motivated by practical energy payoffs through cost-shared collaborations with industry. The areas emphasized in the research portfolio are high temperature superconducting wires, microfabricated instrumentation for chemical sensing, and radioactive stents to prevent reformation of arterial blockage.

Pacific Northwest National Laboratory

Pacific Northwest National Laboratory (PNNL) is a Multiprogram Laboratory located on 640 acres at the Department's Hanford site in Richland, Washington. The MICS subprogram at PNNL conducts basic research in the mathematics and computer science, as well as research in advanced computing software tools and collaborative tools. PNNL also participates in several scientific application pilot projects and participates on a number of the SciDAC teams. The LTR subprogram at PNNL conducts research motivated by practical energy payoffs through cost-shared collaborations with industry. The areas emphasized in the research portfolio are mathematical simulations of glass production, interactions of biological polymers with model surfaces, and characterization of microorganisms in environmental samples.

Princeton Plasma Physics Laboratory

The Princeton Plasma Physics Laboratory (PPPL), a laboratory located in Plainsboro, New Jersey, is dedicated to the development of magnetic fusion energy. The LTR subprogram at PPPL conducts research in areas that include the plasma processing of semiconductor devices and the study of beam-surface interactions through cost-shared collaborations with industry.

Sandia National Laboratories

Sandia National Laboratories (SNL) is a Multiprogram Laboratory, with a total of 3,700 acres, located in Albuquerque, New Mexico, with sites in Livermore, California, and Tonopah, Nevada. The MICS subprogram at SNL conducts basic research in mathematics and computer science, as well as research in advanced computing software tools and collaborative tools. SNL also participates in several scientific application and collaborative pilot projects and participates on a number of the SciDAC teams.

Stanford Linear Accelerator Center

The Stanford Linear Accelerator Center (SLAC) is located at the edge of Silicon Valley in California about halfway between San Francisco and San Jose on 426 acres of Stanford University land. The LTR subprogram at SLAC conducts research in areas such as advanced electronics, large-scale ultra-high vacuum systems, radiation physics and monitoring, polarized and high-brightness electron sources, magnet design and measurement, and controls systems through cost-shared collaborations with industry.

Thomas Jefferson National Accelerator Facility

The Thomas Jefferson National Accelerator Facility (TJNAF) is a basic research laboratory located on a 200 acre site in Newport News, Virginia. The LTR subprogram at the TJNAF conducts research in such areas as accelerator and detector engineering, superconducting radiofrequency technology, speed data acquisition, and liquid helium cryogenics through cost-shared collaborations with industry.

All Other Sites

The ASCR program funds research at 71 colleges/universities located in 24 states supporting approximately 126 principal investigators. Also included are funds for research awaiting distribution pending completion of peer review results.

A number of Integrated Software Infrastructure Centers will be established at laboratories and/or universities. Specific site locations will be determined as a result of competitive selection. These centers will focus on specific software challenges confronting users of terascale computers.

Mathematical, Information, and Computational Sciences

Mission Supporting Goals and Measures

The Mathematical, Information, and Computational Sciences (MICS) subprogram is responsible for carrying out the primary mission of the ASCR program: discovering, developing, and deploying advanced scientific computing and communications tools and operating the high performance computing and network facilities that researchers need to analyze, model, simulate, and — most importantly — predict the behavior of complex natural and engineered systems of importance to the Office of Science and to the Department of Energy.

The computing and the networking required to meet Office of Science needs exceed the state-of-the-art by a wide margin. Furthermore, the algorithms, software tools, the software libraries and the software 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, to develop software tools, software libraries and software environments. Results from enabling research supported by the MICS subprogram are used by computational scientists supported by other Office of Science and other 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 to researchers working on problems relevant to DOE's scientific missions 24 hours a day, 365 days a year.

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 (17) awards were made. The goal of the ECPI activity is to support Office of Science 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.

ACCOMPLISHMENTS

- **ParamBench demonstrates the significant impact of concurrent memory accesses** - Computer scientists at the Lawrence Livermore National Laboratory, in collaboration with researchers at the University of Utah and North Carolina State University have implemented ParamBench, low-level benchmarks of memory performance in symmetric multiprocessors (SMPs). These benchmarks measure the raw memory performance of SMPs, including the effect of multiple processors accessing the memory system concurrently. Results with this benchmark suite demonstrate that standard latency-hiding techniques, such as hardware prefetching, are less effective in SMPs, even with a crossbar-based memory interconnection.
- **New Analysis Tools for Innovative Materials** - Mathematicians at the Oak Ridge National Laboratory have extended the class of materials science problems that can be solved by a powerful technique known as the "Boundary Element Method." This numerical method significantly

reduces the number of operations that are needed to solve materials science problems, but has traditionally been applicable only to homogeneous materials. The researchers derived the fundamental solution to a set of integral equations for "Functionally Graded Materials," an important class of materials that are not homogeneous, but whose properties vary smoothly. These materials already play an important role in many applications, including coatings for protecting turbine blades, special optical materials, and dental implants and other bio-materials.

- **Scientific Data Objects: A Common Language for Exchanging Parallel Data** - Arrays, or matrices, are one of the basic data structures of scientific computing. In large-scale simulations, arrays are often so large that they must be distributed across many processors. In order for different software modules to work together on a distributed array, a method must exist to precisely describe the distribution of the data. As part of the SciDAC Center for Component Technology for Simulation Software, researchers at the Oak Ridge National Laboratory developed such a description, thus greatly simplifying the development of components that need to exchange distributed array data objects with other components. The new interface specification is capable of describing the layouts used by a wide range of distributed array tools, including CUMULVS (ORNL), Global Arrays (PNNL), High Performance Fortran, A++/P++ (LLNL), and others.
- **New Scientific Data Index Performs 100 Times Faster Than Commercial Database Systems** - Terascale computing and large scientific experiments produce enormous quantities of data that require effective and efficient management. The task of managing scientific data is overwhelming. Researchers at the Lawrence Berkeley National Laboratory have developed a specialized index for accessing very large datasets that contain a large number of attributes that may be queried. This new index performs 12 times faster than the previous best-known method, and 100 times faster than conventional indexing methods in commercial database systems. The prototype index is being used by researchers in high energy physics and combustion modeling.
- **Faster Reconstruction Methods are Making Waves** - Mathematicians at the Lawrence Berkeley National Laboratory have developed efficient and fast techniques for solving the problem of multiple arrivals; that is, detecting and separating the arrival of waves that have taken differing paths through a medium. Example applications include geophysical analysis, which is important for oil exploration, and antenna design. The methods are fast enough that they can be embedded inside "inverse solvers," computer codes that use information about the arriving waves to deduce the characteristics of an unknown body between the source and detector. This will result in new computational tools to examine hidden objects, accurately reconstruct inaccessible regions, and rapidly test proposed models.
- **Increasing Scientific Productivity through Automated Optimization** - Many complex problems in science, engineering and business require the solution of optimization problems, but the conventional approach to solving such problems can be extremely time-consuming and difficult to apply. Researches at Argonne National Laboratory have developed the Network-Enabled Optimization System (NEOS) that allows users to solve optimization problems over the Internet with state-of-the-art software and without tedious downloading and linking of specialized optimization code. Because of its ease of use, the NEOS server has gained widespread popularity with more than 5,000 job requests each month from users around the world. Recent NEOS applications include circuit simulation, protein folding, circuit design, brain modeling, airport crew scheduling, and modeling of electricity markets.

- **OSCAR Cluster Software Distribution A Big “Hit” Worldwide** - The Open Source Cluster Application Resources package, OSCAR, is a collection of software tools for managing Linux-based computer clusters developed by a consortium of academic, research, and industry members led by scientists at the Oak Ridge National Laboratory. According to the Top 500 Clusters web site, OSCAR has become the most used cluster computing distribution available today. OSCAR is also used as the core cluster base package in the MacNeil Schwindler (MSC) Linux commercial cluster distribution as well as the NCSA “in-a-box” series of cluster computing solutions. OSCAR has a “market share” of over 30% according to the poll – more than twice its nearest competitor. OSCAR has been downloaded over 53,000 times and has received over 140,000 web page hits during the past year.
- **Tiled Displays: Automatic Calibration of Scalable Display Systems** - Today’s scientific simulations and rich multimedia collaborative environments can easily produce many millions to tens of millions of pixels for display. Tiled display systems built by combining the images from arrays of projectors can provide massive numbers of pixel elements to visually represent large amounts of information. Multiprojector tiled arrays can be a cost-effective way to create these displays, and they may be the only practical way to create large information dense displays. But, it is difficult to create the illusion of a unified seamless display for a variety of reasons, including projector-to-projector color and luminosity differences, variation of luminosity across the image from a single projector, and optical distortion of the individual projector images caused by imperfections in the lenses and misalignment of projectors. Researchers at Argonne National Laboratory have developed methods to attack these fundamental issues which provide an efficient and optimized measurement process using inexpensive components that is tolerant of a wide range of imperfections in components and measurement setup such as lighting conditions and camera optics.
- **NERSC Improves Supercomputer Performance.** The Department of Energy's National Energy Research Scientific Computing (NERSC) Center at the Lawrence Berkeley National Laboratory has improved the utilization of its 5 Tflops supercomputer, NERSC-3. After only six months of operation, NERSC-3 began to deliver 90-95% of its cycles to users, on a routine basis.
- **ESnet deploys next general protocol** – ESnet has deployed Internet Protocol Version 6 (IPv6) on its production network. Enabling IPv6 on the network brings a new level of security (e.g. packet encryption and source authentication) and supports real-time traffic, such as video conferencing. IPv6 is expected to become the protocol of choice throughout the Internet.

AWARDS

Top Young Innovator Award – A computer scientist at Argonne National Laboratory has been named one of the world's top 100 young innovators by Technology Review, MIT's Magazine of Innovation. The list recognizes 100 individuals under the age of 35 whose innovative work in business and technology is having a profound influence on today's world. This scientist’s work centers on development of Grid technologies for connecting geographically dispersed resources. He also leads standardization efforts of the Globus Project™.

Scientific Computing Research Investments

High-performance computing hardware is important for meeting DOE's modeling and simulation needs. However, computer hardware can only enable scientific advances when the appropriate algorithms, scientific software tools, libraries, software environments, and the networking infrastructure are easy to use and are readily available to the users. The MICS subprogram differs from high performance computing efforts in other Federal agencies because of its management focus to integrate research investments to enable new science. Desktop systems realize advances in computing power primarily through increases in the processor's clock speed. High performance computers employ a different strategy for achieving performance, complicating the architecture and placing stringent requirements on software. The MICS subprogram supports software research over a broad range, but that research is tailored to DOE's science needs. Research is underway to improve the performance of simulations on high-end computers, to remove constraints on the human-computer interface and to discover the specialized information management and analysis techniques that scientists need to manage, analyze and visualize extremely large data files.

Technology trends and business forces in the U.S. computer system industry over the past decade caused most domestic vendors to curtail or abandon the development of high-end systems designed to meet the most demanding requirements of scientific research. Instead, large numbers of smaller commercial systems were combined and integrated into terascale computers to achieve the peak performance levels required for agency missions in computational science. The hardware is complicated, unwieldy and not balanced for scientific applications. Enabling software has been developed for scientists to take advantage of these new computers. However, this software is extraordinarily complex. Consequently, the DOE, primarily through the MICS subprogram, and other Federal agencies whose missions depend on high-performance computing, must make basic research investments to adapt high-performance computing and networking hardware into tools for scientific discovery.

To make progress in the future, our current strategy needs to be adjusted. Continued emphasis on developing software-based solutions to enable scientific simulations on large clusters of computers designed for mid-range applications is no longer the basis for a sustainable strategy for many high-end applications. Rather, our emphasis needs to broaden to include computer hardware technology, architecture, and design trends motivated from a scientific user perspective. This can be accomplished by making research investments that couple computational scientists and computer scientists with U.S. computer vendors to orient future computer architectures towards the need of science. Additional research investments would be made to ensure that the software takes full advantage of the computer architecture. The status of the technology, the conditions of the current business market for computing, and the success of the Earth Simulator supercomputer in Japan are strong indicators that this strategy will provide tangible near-term results for scientific simulation. This revised strategy is the tenet for the NGA effort. While NGA will be instrumental in removing architectural bottlenecks to performance on actual scientific simulations, others will remain and possibly become persistent obstacles in the future.

To illustrate the complexities involved, think of a high-performance computer as a large number of conference rooms distributed around a region. Each conference room is connected through the region's transportation and communications infrastructure. Now, the task of a successful scientific application is analogous to getting everyone in the region to a pre-assigned conference room on time. Instructions are given to each participant (systems software). Results from each conference (calculations) will be

documented (stored in memory) for distribution. New conferences are convened, new instructions are given and new decisions are made. Now repeat this process trillions of times, as occurs in a scientific simulation! As one can appreciate, this process can only work if the region's infrastructure is properly configured and operating efficiently. That is, the buses, subways, taxicabs, roads, elevators and telephones can efficiently handle the demand. Most of the systems available from computer vendors are analogous to small regions, a limited number of conference rooms and an inefficient infrastructure. Computers for scientific simulation on the other hand, must be analogous to large cities, large numbers of conference rooms, and an efficient infrastructure, with alternative modes of transportation and communication.

Advances in *computer science* research can enable scientists to overcome these remaining barriers. For example,

- efficient, high-performance operating systems, compilers, and communications libraries for high-end computers;
- software to enable scientists to store, manage, analyze, visualize, and extract scientific understanding from the enormous (terabyte to petabyte) data archives that these computers will generate;
- software frameworks that enable scientists to reuse most of their intellectual investment when moving from one computer to another and make use of lower-level components, such as runtime services and mathematical libraries, that have been optimized for the particular architecture;
- scalable resource management and scheduling software for computers with thousands of processors;
- performance monitoring tools to enable scientists to understand how to achieve high performance with their codes; and
- provide computational scientists with tools, options, and strategies to obtain the maximum scientific benefit from their computations.

Research advances in computer science do not provide the full range of capabilities that computational scientists need, especially for the complex problems faced by the Office of Science. Significant efforts in the applied mathematical research activity will be required for the Department to satisfy its mission requirements for computational science. Historically, improvements in mathematical algorithms have yielded at least as much increase in performance as have improvements in hardware. A large proportion of these advances resulted from the MICS subprogram applied mathematics research activity. The requirements of scientific domains for new algorithms that can scale to work effectively across thousands of processors and produce the most science in the fewest number of computer operations drives the need for improved mathematical algorithms and the supporting software libraries that must be made available for ready use by scientists. In this area of research, the MICS applied mathematics activity is the core of the nationwide effort.

The MICS subprogram research activities that respond to these challenges are described below in the Detailed Program Justification section of the MICS subprogram budget under the headings:

- Applied Mathematics
- Computer Science
- Advanced Computing Software Tools

High Performance Networking, Middleware and Collaboratory Research Investments

Advances in network capabilities and network-enabled technologies now make it possible for large geographically distributed teams to effectively collaborate on solutions to complex problems. It is now becoming possible to harness and integrate the collective capabilities of large geographically distributed data archives, research teams, and computational resources. This collective capability is especially important for the teams using the major experimental facilities, computational resources, and data resources supported by DOE because all of the necessary resources are not available at one location. To successfully realize the potential of this collective research capability, additional research is needed to bring network, data, and computational resources to the members of a distributed team in a manner that is easy to use and guarantees end-to-end performance. For example:

- Significant research is needed to augment the capability of the Internet to support distributed high-end data-intensive applications and to secure large-scale scientific collaborations. The requirements of high-performance networks that support distributed data-intensive computing and scientific collaborations on a national and international scale are very different than the requirements of the current commercial networks where millions of users are moving small web pages. The MICS-supported research on high-performance networks includes research on high-performance protocols, network-aware operating system services, advanced network coprocessors, network measurement and analysis.
- Research is also needed for the development and testing of high-performance middleware needed to seamlessly couple scientific applications to the underlying transport networks. These include high-performance middleware such as advanced security services for grid computing, ultra-high-speed data transfer services, services to guarantee Quality of Service (QoS) for delay sensitive applications, and grid resources discovery. This high-performance middleware provides the scalable software components needed to integrate data, visualization, computation and high-speed networks into a scalable and secure scientific collaborative environment.

The MICS subprogram will address these challenges through fundamental research in networking; software tools that integrate networking and computer science to enable scientific collaboration (collaboratory tools); partnerships with key scientific disciplines; and advanced network testbeds.

Specific responses to these challenges are described in the Detailed Program Justification section of the MICS subprogram budget under the headings:

- Networking
- Collaboratory Tools
- National Collaboratory Pilot Projects

Enhancements to High Performance Computing and Networking Facilities

To realize the scientific opportunities offered by advanced computing, enhancements to the Office of Science's computing and networking facilities are also required. The MICS subprogram supports a suite of high-end computing resources and networking resources for the Office of Science:

- **Production High Performance Computing Facilities.** The National Energy Research Scientific Computing Center (NERSC) provides high performance computing for investigators supported by

the Office of Science. NERSC provides a spectrum of supercomputers offering a range of high performance computing resources and associated software support.

- **Energy Sciences Network (ESnet).** ESnet provides worldwide access to Office of Science facilities, including light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, high-end computing facilities, massive data resources and other leading-edge instruments and facilities.
- **Advanced Computing Research Testbeds.** The Advanced Computing Research Testbeds (ACRTs) consist of high performance, advanced architecture computing platforms for testing and evaluation to ascertain the prospects for meeting future general, or specialized, computational science needs of the Office of Science. In FY 2004, the ACRTs will provide hardware resources for the NGA activity. Two types of computing platforms will be evaluated - early systems from vendors, and experimental systems. Based on an analysis of vendor offerings and a peer review of the potential that such offerings can meet Office of Science computational needs, hardware will be acquired at sufficient scale to address key performance and software scaling issues. The evaluation process will include computer science studies and tests of leading-edge Office of Science computational science applications, such as those being developed under SciDAC. In addition, the ACRTs will provide computing resources to SciDAC teams.
- **Trends for Future Supercomputing and Networking Resources.** The need for high performance computational resources will increase in future years as applications transition from the software development and testing phase to using the software to generate new science. As the peak performance of the computers increase, the amount of data produced in a simulation increases as well. Therefore, focused enhancements to the Office of Science's network infrastructure are required to enable scientists to access and understand the data generated by their software and by large-scale science experiments.

The MICS subprogram activities that respond to these challenges are described later in the Detailed Program Justification section of the MICS subprogram budget under the headings:

- National Energy Research Scientific Computing Center (NERSC)
- Advanced Computing Research Testbeds
- Energy Sciences Network (ESnet)

Subprogram Goals

The MICS subprogram goals are identical to the ASCR program goals, and the performance indicators and targets for ASCR apply directly to the activities of the MICS subprogram. Therefore, no subprogram goals are included in the MICS section of the ASCR budget.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	\$ Change	% Change
Mathematical, Computational, and Computer Sciences Research.....	52,877	75,633	83,300	+7,667	+10.1%
Advanced Computation, Communications Research and Associated Activities	94,282	83,782	82,591	-1,191	-1.4%
SBIR/STTR	0	4,142	4,599	+457	+11.0%
Total, Mathematical, Information, and Computational Sciences.....	147,159	163,557	170,490	+6,933	+4.2%

Detailed Program Justification

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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Mathematical, Computational, and Computer Sciences Research.....

	52,877	75,633	83,300
■ Applied Mathematics.....	22,655	23,141	22,634

This activity supports research on the underlying mathematical understanding of physical, chemical and biological systems, and on advanced numerical algorithms that enable effective description and prediction of such systems on terascale computing systems. Research in Applied Mathematics supported by MICS underpins computational science throughout DOE. Historically, the numerical algorithms developed under this activity have produced more scientific advances through simulation than 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 solutions 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); and automated reasoning systems.

The FY 2004 budget continues the Computational Sciences Graduate Fellowship program at the current level of \$3,500,000.

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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The decrease in funding for this activity between FY 2003 and FY 2004 includes the transfer of Genomes to Life activities to Scientific Application Partnerships to better reflect the character of the research. In FY 2003, \$1,491,000 was transferred to the Department of Homeland Security for evaluation of applied mathematical sciences activities at the Lawrence Livermore National Laboratory to determine which are most suitable for transfer to the Department of Homeland Security.

■ **Computer Science** **19,517** **17,506** **23,680**

This activity supports research in computer science to enable researchers to effectively utilize high-performance computers 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. 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 under circumstances where the underlying resources and users are geographically distributed. The first area includes research in protocols and tools for interprocessor communication and parallel input/output (I/O) as well as tools to monitor the performance of scientific applications and advanced techniques for visualizing very large-scale scientific data. Researchers at DOE laboratories and universities, often working together in partnerships, propose and conduct this research.

In FY 2003, \$1,491,000 was transferred to the Department of Homeland Security for evaluation of computer science activities at the Lawrence Livermore National Laboratory to determine which are most suitable for transfer to the Department of Homeland Security. *In addition, the FY 2004 budget includes \$4,659,000 for an academic and domestic computer vendor research effort on future generation operating systems and runtime environments. Critical goals for this NGA effort will be to enable future operating systems runtime environments to deliver maximum performance to scientific applications. Projects will be competitively selected.*

■ **Advanced Computing Software Tools** **5,543** **20,256** **20,256**

This activity supports research that builds on the results from research in applied mathematics and computer science to develop integrated software tools that computational scientists can use to develop high performance 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 high-end computing systems.

In FY 2004, this activity will continue to support the Integrated Software Infrastructure Centers (ISICs), a SciDAC activity, competitively selected in FY 2001. The ISICs funded under this activity focus on: 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

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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development of data management and visualization software capable of handling terabyte scale data sets extracted from petabyte scale data archives, and software for managing computers with thousands of processors; and software component technology to enable rapid development of efficient, portable, high performance parallel simulation software.

These Integrated Software Infrastructure Centers are a critical 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 to be maintained, bug-free and upgraded, as necessary. Software for tools high performance scientific simulations have no commercial market. The Integrated Software Infrastructure Centers initiated in FY 2001 provide the only means for developing and deploying these tools to the scientific community.

■ **Scientific Applications Partnerships** **5,162** **14,730** **16,730**

This activity, formerly titled Scientific Application Pilot Projects, supports collaborative research with disciplinary computational scientists to apply the computational techniques and tools developed by other MICS activities to address problems relevant to the mission of SC. 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 2004 funding for this activity will allow the continuation of the partnerships that were competitively selected in FY 2001. These projects are part of the SciDAC activity and are coupled to the Integrated Software Infrastructure Centers. 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.

The FY 2004 request includes funds to continue the partnership with the Biological and Environmental Research program Genomes to Life and the partnership with the Basic Energy Sciences program in nanoscale science. *The FY 2004 in request also includes \$2,000,000 to support research under the NGA to understand the relationship among programming models, architecture features and application performance. Projects will be selected through a peer reviewed, open competition.*

Advanced Computation, Communications Research, and Associated Activities **94,282** **83,782** **82,591**

■ **Networking** **7,329** **7,066** **7,066**

This activity supports research and development in high-performance networks needed to develop and deploy advanced networking capabilities to address challenging issues such as ultra-high-speed data transfers, remote visualization, real-time remote instrumentation, and large-scale scientific collaboration. Networking research is carried out at national laboratories and universities and consists of two major elements:

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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Network R&D – to address the fundamental issues of high-performance networks to support access to the next generation of scientific facilities, terascale computing resources and distributed petabyte-scale data archives. Network R&D focuses on leading-edge networking technologies such as ultra optical transport protocols and services for ultra high-speed data transfers; techniques and tools for ultra high-speed network measurement and analysis; advanced network tools and services to enable network-aware, high-end scientific applications; and scalable cyber-security technologies for open science environment.

Advanced experimental networking – to accelerate the adoption of emerging networking technologies and to transfer networking R&D results into production networks that support science applications. It includes activities such as experimental networking testbeds, advanced deployment and evaluation of new networking technologies, and exploration of advanced networking concepts. A rapid adoption of emerging network capabilities into production networks will enable scientists pushing the limits of today’s networks capabilities to use networking technologies to conduct far-reaching experiments.

■ **Collaboratory Tools** **7,000** **5,527** **5,527**

This activity supports research that builds on results of fundamental research in computer science and networking to develop an integrated set of software tools to support scientific collaborations. This includes enabling scientists to remotely access and control facilities and share data in real time, and to effectively share data with colleagues throughout the life of a project. These tools provide a new way of organizing and performing scientific work that offers the potential for increased productivity and efficiency and will also enable broader access to important DOE facilities and data resources by scientists and educators throughout the country. It is particularly important to provide for efficient, high-performance, reliable, secure, and policy-aware management of large-scale data movement. This research includes an effort to develop a set of essential middleware services required to support large-scale data-intensive collaboratory applications. This research also includes an effort to research, develop, and integrate the tools required to support a flexible, secure, seamless collaboration environment that supports the entire continuum of interactions between collaborators. The goal is to seamlessly allow collaborators to locate each other, use asynchronous and synchronous messaging, share documents, progress, results, applications and hold videoconferences. There is also research for developing and demonstrating an open, scalable approach to application-level security in widely distributed, open network environments that can be used by all the collaboratory tools as well as by the advanced computing software tools whenever access control and authentication are issues.

■ **National Collaboratory Pilot Projects**..... **9,384** **10,857** **10,857**

This activity supports research that tests, validates, and applies collaboratory tools in real-world situations in partnership with other DOE programs. The competitively selected partnerships involve national laboratories, universities, and U.S. industry. It is important to continue to demonstrate and test the benefits of collaboratory tools technology in order to promote its widespread use and enable more effective access to the wide range of resources within the

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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Department, from light sources to terascale computers to petabyte data storage systems. The partnerships that were initiated in FY 2001 focus on developing user environments where collaboration is ubiquitous and distributed computing is seamless and transparent for DOE mission applications. The Particle Physics Data Grid is developing middleware infrastructure to support High Energy Physics (HEP) and Nuclear Physics (NP) communities, and to enable grid-enabled data-management ("manipulation") and analysis capabilities "at the desk of every physicist." It is building one unified system that will be capable of handling the capture, storage, retrieval and analysis of particle physics experiments at the five most critical research facilities, a key collaboratory issue being the highly distributed access to, and processing of, the resulting data by a worldwide research community. In another community, the Earth System Grid II is developing a virtual collaborative environment linking distributed centers, models, data, and users that will facilitate exchange among climatologists all over the world and provide a needed platform for the management of the massive amounts of data that are being generated. Development of this and similar concepts is essential for rapid, precise, and convincing analysis of short- and long-term weather patterns, particularly in the period when increasing pollution introduces changes that may affect us for generations to come. The National Fusion Collaboratory is centered on the integration of collaborative technologies appropriate for widely dispersed experimental environments and includes elements of security, distributed systems, and visualization. All three of these pilot collaboratories will rely on the DOE Science Grid to provide the underpinnings for the software environment, the persistent grid services, that make it possible to pursue innovative approaches to scientific computing through secure remote access to online facilities, distance collaboration, shared petabyte datasets and large-scale distributed computation.

■ **National Energy Research Scientific Computing Center (NERSC)** **31,244 28,244 28,244**

NERSC, located at LBNL, provides high performance computing for investigators supported by the Office of Science. The Center serves 2,400 users working on about 700 projects; 35 percent of users are university based, 61 percent are in National Laboratories, 3 percent are in industry, and 1 percent in other government laboratories. The major computational resource at NERSC is an IBM SP computer. The initial installation of hardware, which was completed in FY 2001 following a fully competitive process, provided a peak performance of 5 trillion floating point operations per second (teraflops) to its users. The capability of this system was increased to 10 teraflops following the acquisition of additional computer hardware in FY 2003. The FY 2004 funding will support the continued operation of the IBM SP computer at 10 teraflops peak performance. These computational resources are integrated by a common high performance file storage system that facilitates interdisciplinary collaborations. Related requirements for capital equipment, such as high-speed disk storage systems, archival data storage systems, and high performance visualization hardware, and general plant projects (GPP) funding are also supported. FY 2004 capital equipment requirements remain at the same level as in FY 2003.

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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■ **Advanced Computing Research Testbeds (ACRTs)..... 20,295 15,300 12,609**

This activity supports the acquisition, the testing and the evaluation of advanced computer hardware testbeds to assess the prospects for meeting future computational needs of the Office of Science, such as SciDAC and special purpose applications. The ACRT activity will provide two types of computer testbeds for evaluation - early systems and experimental systems. Each testbed will involve significant research and architecture design activities. *The FY 2004 request includes \$7,309,000 to complete the evaluation of Cray X1 hardware that was initiated in FY 2002. The reduction in this activity will allow the program to focus on a single new evaluation under the NGA and provide critical resources to SciDAC teams.*

■ **Energy Sciences Network (ESnet)..... 19,030 16,788 18,288**

ESnet is a high-performance network infrastructure that supplies 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 Office of Science 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. 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 provides interfaces between the network fabric it provides and peering arrangements with 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. In FY 2004, funds will be used to operate ESnet and to continue support for upgrading the capability of the ESnet backbone to 10,000 million bits per sec (Mbps) from its current capability of 155 Mbps. Remaining funds will be used to upgrade networking hardware and services at high priority ESnet sites to exploit the enhanced performance capabilities of the backbone.

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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SBIR/STTR..... 0 4,142 4,599

In FY 2002, \$3,656,000 and \$220,000 were transferred to the SBIR and STTR programs, respectively. The FY 2003 and FY 2004 amounts are the estimated requirement for the continuation of the SBIR and STTR program.

Total, Mathematical, Information, and Computational Sciences 147,159 163,557 170,490

Explanation of Funding Changes

FY 2004 vs. FY 2003 (\$000)

Mathematical, Computational, and Computer Sciences Research

- **Applied Mathematics.** The decrease results from the transfer of Genomes to Life activities to Scientific Application Partnerships to better reflect the character of the research, partially offset by increases to core Applied Mathematics research. Funding for Homeland Security in FY 2003 is budgeted by the Department of Homeland Security in FY 2004..... -507
 - **Computer Science.** Provides an increase under the NGA for an academic and domestic computer vendor research effort. Includes an increase to provide core research infrastructure for NGA. Funding provided for Homeland Security in FY 2003 is budgeted by the Department of Homeland Security in FY 2004. +6,174
 - **Scientific Application Partnerships.** Provides an increase to support research under the NGA to understand the relationship among programming models, architecture features and application performance..... +2,000
- Total Mathematical, Computational, and Computer Sciences Research..... +7,667

Advanced Computation, Communications Research, and Associated Activities

- **Advanced Computing Research Testbed.** Reduction in this program to focus on single new evaluation under the NGA and providing critical resources to SciDAC teams..... -2,691
 - **ESnet.** Provides an increase in this program element for upgrades to the ESnet infrastructure for an architecture tailored to a class of applications within the SciDAC research portfolio to produce new science..... +1,500
- Total Advanced Computation, Communications Research, and Associated Activities..... -1,191

FY 2004 vs. FY 2003 (\$000)

SBIR/STTR

■ Increase in SBIR/STTR due to increase in operating expenses	<u>+457</u>
Total Funding Change, Mathematical, Information, and Computational Sciences	<u>+6,933</u>

Laboratory Technology Research

Mission Supporting Goals and Objectives

The Laboratory Technology Research (LTR) subprogram is being brought to a successful conclusion in FY 2004. The mission of the Laboratory Technology Research subprogram is to support high-risk research that advances science and technology to enable applications that could significantly impact the Nation's energy economy. LTR fosters the production of research results motivated by a practical energy payoff through cost-shared collaborations between the Office of Science (SC) laboratories and industry.

An important component of the Department's strategic goals are to ensure that the United States maintains its leadership in science and technology. LTR is the lead program in the Office of Science for leveraging science and technology to advance understanding and to promote our country's economic competitiveness through cost-shared partnerships with the private sector.

The National Laboratories under the stewardship of the Office of Science conduct research in a variety of scientific and technical fields and operate unique scientific facilities. Viewed as a system, these ten laboratories — Ames Laboratory, Argonne National Laboratory, Brookhaven National Laboratory, Fermi National Accelerator Laboratory, Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Princeton Plasma Physics Laboratory, Stanford Linear Accelerator Center, and Thomas Jefferson National Accelerator Facility — offer a comprehensive resource for research collaborations. The major component of the LTR research portfolio consists of investments at these laboratories to conduct research that benefits all major stakeholders — the DOE, the industrial collaborators, and the Nation. These investments are further leveraged by the participation of an industry partner, using Cooperative Research and Development Agreements (CRADAs). Another LTR subprogram component provides funding to the Office of Science national laboratories to facilitate rapid access to the research capabilities at the SC laboratories through agile partnership mechanisms including personnel exchanges and technical consultations with small business. The LTR subprogram currently emphasizes four critical areas of DOE mission-related research: advanced materials processing and utilization, nanotechnology, intelligent processes and controls, and energy-related applications of biotechnology.

Funding Schedule

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	\$ Change	% Change
Laboratory Technology Research.....	3,046	2,921	2,916	-5	-0.2%
SBIR/STTR.....	0	79	84	+5	+6.3%
Total, Laboratory Technology Research .	3,046	3,000	3,000	0	--

Detailed Program Justification

(dollars in thousands)

FY 2002	FY 2003	FY 2004
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Laboratory Technology Research	3,046	2,921	2,916
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This activity supports research to advance the fundamental science at the Office of Science (SC) laboratories toward innovative energy applications. Through CRADAs, the SC laboratories enter into cost-shared research partnerships with industry, typically for a period of three years, to explore energy applications of research advances in areas of mission relevance to both parties. The research portfolio consists of 12 projects and emphasizes the following topics: advanced materials processing and utilization, nanotechnology, intelligent processes and controls, and energy-related applications of biotechnology. Efforts underway include the exploration of (1) new cast steels with microstructures and mechanical properties better than comparable cast alloys, to provide an improved critical component material for higher efficiency steam and gas turbine technology for electric power generation; (2) radiative carrier recombination in group-III nitride thin films, to optimize the performance of GaN-based high-brightness Light Emitting Diodes for applications in energy-efficient lighting; and (3) molecular structures of new classes of hydrophorphyrin photosensitizers for use with light and oxygen to destroy cancerous cells and tissues. A small but important component of this activity provides industry, particularly small businesses, with rapid access to the unique research capabilities and resources at the SC laboratories. These research efforts are usually supported for a few months to quantify the energy benefit of a specific problem posed by industry. Recent projects supported the development of: (1) an economically-viable duplex chromium nitride near-frictionless carbon film capable of providing extreme wear resistance and reduced friction to sliding engine and drive train components in advanced diesel engines; (2) a detailed understanding of the interplay between platinum/cadmium zinc telluride interfacial chemistry and radiation detector performance for applications such as finding new cancer locations; and (3) an ion source for producing negative heavy ions for ion implantation in the semiconductor industry, which will eliminate toxic gas.

SBIR/STTR	0	79	84
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In FY 2002, \$75,000 and \$4,000 were transferred to the SBIR and STTR programs, respectively. The FY 2003 and FY 2004 amounts are the estimated requirement for the continuation of the SBIR and STTR program.

Total, Laboratory Technology Research	3,046	3,000	3,000
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Explanation of Funding Changes

FY 2004 vs. FY 2003 (\$000)

There are no significant funding changes.

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

(dollars in thousands)

	FY 2002	FY 2003	FY 2004	\$ Change	% Change
General Plant Projects.....	0	1,000	0	-1,000	-100.0%
Capital Equipment (total)	3,777	6,250	6,250	0	--
Total, Capital Operating Expenses	3,777	7,250	6,250	-1,000	-13.8%