# Advanced Scientific Computing Research

## Program Mission

The mission of the Advanced Scientific Computing Research (ASCR) program is to foster and support fundamental research in advanced scientific computing – applied mathematics, computer science, and networking and provide the high performance computational and networking tools that enable DOE to succeed in its science, energy, environmental quality, and national security missions. The importance of advanced scientific computing to the missions of the Department was clearly stated in the "Scientific Discovery through Advanced Computing," (SciDAC) report, which was delivered to Congress in March 2001:

> *"Advanced scientific computing is key to accomplishing the missions of the U.S. Department of Energy (DOE). It is essential to the design of nuclear weapons, the development of new energy technologies, and the discovery of new scientific knowledge. All of the research programs in DOE's Office of Science … have identified major scientific questions that can only be addressed through advances in scientific computing."*

## Strategic Objectives

SC5: To enable advances and discoveries in DOE science through world-class research in applied mathematics, computer sciences, networks and computational sciences and through the distributed operation of high performance, scientific computing and network facilities; and to deliver, in FY 2006, a suite of specialized software tools for DOE scientific simulations that take full advantage of terascale computers and high speed networks.

SC7-5: Provide major advanced scientific user facilities where scientific excellence is validated by external review; average operational downtime does not exceed 10% of schedule; construction and upgrades are within 10% of schedule and budget; and facility technology research and development programs meet their goals.

## Program Strategic Performance Goals and Targets

**SC5-1:** Build leading research programs in focused disciplines of applied mathematics, computer science, and network and collaboratory 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

Invited presentations at major national and international conferences.

### Performance Standards

As discussed in Corporate Context/Executive Summary.

## Annual Performance Results and Targets

| FY 2001 Results | FY 2002 Targets | FY 2003 Targets |
|---|---|---|
| Initiated project to understand the advantages and issues associated with lightweight kernel operating systems rather than full kernels for the compute nodes of extreme-scale scientific computers. [Met Goal] | Complete 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) | 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) |
| Supported the Computational Science Graduate Fellowship Program with the successful appointment of 20 new students to support the next generation of leaders in computational science for DOE and the Nation. [Met Goal] | Appoint 20 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) | Appoint 20 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) |

**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 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

Software released to applications teams.

### Performance Standards

As discussed in the Corporate Context/Executive Summary.

## Annual Performance Results and Targets

| FY 2001 Results | FY 2002 Targets | FY 2003 Targets |
| --- | --- | --- |
| Operated facilities, including the National Energy Research Scientific Computing Center (NERSC) and ESnet, within budget while meeting user needs and satisfying overall SC program requirements where, specifically, NERSC delivered 3.6 Teraflop capability at the end of FY 2001 to support DOE's science mission. [Exceeded Goal] | Achieve 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)<br><br>Migrate the users with the largest allocations to the IBM-SP from the previous generation Cray T3E. (SC5-2) | Begin installation of next generation NERSC computer, NERSC-4, that will quadruple the capability available to solve leading edge scientific problems. (SC5-2) |
| | | 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 Biological and Environmental Research and Basic Energy Sciences programs, respectively, of submitted proposals. (SC5-2) |

**SC7-5**: Provide advanced scientific user facilities where scientific excellence is validated by external review; average operational downtime does not exceed 10% of schedule; construction and upgrades are within 10% 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.

### Performance Standards

As discussed in the Corporate Context/Executive Summary.

## Annual Performance Results and Targets

| FY 2001 Results | FY 2002 Targets | FY 2003 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) |
| Initiated the review of ASCR high performance computing facilities by the Advanced Scientific Computing Advisory Committee (ASCAC). [Met Goal] | Deliver preliminary report of ASCAC review of ASCR high performance computing facilities. (SC7-5) | 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) |

## Significant Accomplishments and Program Shifts

The major thrust of the research efforts supported by the ASCR program is to establish the mathematics and computer science foundations and develop the specialized software tools needed to effectively utilize rapidly-evolving, high-performance computing and networking hardware to enable new scientific discoveries across the research portfolio of the Office of Science. Advances in microelectronics continue to fuel dramatic performance improvements in computing and networking technologies. However, commercial market needs and expectations, which are driving those improvements, are dramatically different from the needs and the expectations of the researchers being supported to advance DOE science. Consequently, the DOE and other Federal agencies whose missions depend on high-performance, scientific computing, must make research investments to adapt high-performance computing and networking hardware into tools for scientific discovery. The importance of these tools to the DOE Office of Science mission and the fundamental differences between business, personal and scientific requirements are illustrated by the following examples:

- Intermetallic compounds, such as iron-manganese-cobalt (Fe-Mn-Co), have properties that would be attractive in a wide variety of applications including, transportation, data storage and computer read/write heads. Before many of these applications can be realized, an important fundamental feature to understand is the degree of "exchange bias," which is responsible for the novel magnetic properties of these materials. Scientifically, the "exchange bias" arises when an antiferromagnetic layer such as FeMn pins the orientation of the magnetic moment of an adjacent ferromagnetic layer such as Cobalt. A calculation performed during the summer of 2001 showed, for the first time, that the magnetic structure of the FeMn layer adjacent to the cobalt layer of atoms was fundamentally different from the magnetic structure of pure FeMn material. This dramatic discovery provides important scientific insight into the properties of magnetic materials and suggests that the "design" of materials with unusual magnetic properties may be fostered through supercomputer simulations. Here are some features of the calculation:
  - The researchers performed a simulation of two layers of Fe-Mn-Co containing 2,016 atoms. (About 15,000 atoms would be needed to accurately model all features of this intermetallic material.) In order to predict the magnetic behavior in the interface region, approximately 30 trillion operations (i.e. additions, subtractions, multiplications and divisions) are required for each atom. Furthermore, 48 megabytes (MB) of memory were needed to store critical

data for each atom. The entire calculation required approximately 100 gigabytes (GB) of memory and 60 quadrillion ($60 \times 10^{15}$) operations to complete.

  - To put this in context, a 1GHz desktop workstation would need its memory upgraded by a factor of 1500 to perform this calculation, which would take one year to finish. A more realistic comparison can be made by comparing a run on NERSC-3 with a run on a previous generation supercomputer a Cray T3E (NERSC-2). Using 644 processors on the T3E, the code ran at 347 Gflops and required 2 days to complete. Using 2176 processors on the IBM-SP (NERSC-3) the code achieved 2460 Gflops and required only 6.6 hours to complete.

- Scientific simulations to meet Office of Science missions frequently involve accessing large data files on the order of millions to billions of megabytes (MB) in size. These data files are being generated by measurements, experiments, and simulations at many locations around the world. Reliable access to these data requires investments in high-speed high-bandwidth networks, and in robust, efficient network software. To highlight the special features of these requirements, the supercomputing conference series initiated a Network Bandwidth Challenge in 2000, in which researchers were invited to demonstrate their ability to maximize network performance for their application. In both 2000 and 2001, the first prize for optimal use of the network went to a DOE laboratory-led application. In 2001, the prize-winning application was based on an interactive, scientific simulation running at two separate supercomputers. The results of the simulation were sent to the conference floor over the network and visualized at a sustained network performance level of 3.3 gigabits per second, or approximately 1,000 times faster than commercially available DSL.
- A national consortium of climate scientists, computer scientists and applied mathematicians, including DOE researchers, is developing the Coupled Parallel Climate Model (PCM), a terascale simulation code to assist the U.S. National Assessment effort in global climate change. The PCM code is unique in combining atmospheric, ocean, and sea-ice models into a tightly coupled terascale simulation. The PCM code must be run many times with varying assumptions on environmental conditions to create an ensemble of results that, in the aggregate, provides the capability of predicting trends in global climate change. Today's largest supercomputers and software tools can reliably produce results with about 300 km resolution, which is adequate for simulating global effects, such as the jet stream and the temperature profile of the earth. Next generation supercomputer hardware and software tools will be required to perform simulations on a 50 km resolution or less. This will allow accurate simulation of regional effects, such as complex topography and the influence of rivers and streams.

The ASCR program builds on several decades of leadership in high performance computing and many pioneering accomplishments, such as the establishment of the first national supercomputer center in 1974. The principles that guide the integration of these efforts will be discussed in more detail in the MICS subprogram narrative. Building on this long history, principal investigators have received recognition through numerous prizes, awards, and honors. A list of FY 2001 accomplishments and awards is given below.

## ACCOMPLISHMENTS

### Mathematical, Information and Computational Sciences

- *Babel Language Interoperability: Component Technology for Scientific Software.* Computer scientists at Lawrence Livermore National Laboratory, in collaboration with members of the Common Component Architecture working group, have developed a language interoperability tool that supports the re-use of scientific libraries across multiple programming languages that are prevalent in high end applications. Previously, application developers often could not re-use existing software libraries if the library and the application were written in different programming languages. Using LLNL's language interoperability tool, called Babel, library writers may now deliver libraries that can be called from any of the standard scientific languages, including Fortran 77, C, C++, and Python. Support for Java and Fortran 90 is under development.

- *Hypre: Conceptual Interfaces Provide Access to State-of-the-art Linear Solvers.* A valuable new approach for describing linear systems of equations to linear solver libraries can be described as so-called "physics-based" or "conceptual" interfaces. Unlike traditional matrix-based interfaces used in most libraries, conceptual interfaces are more natural for application users and provide the additional information (e.g., the description of a computational grid) necessary for exploiting powerful linear solver algorithms such as geometric multigrid. Researchers at the Lawrence Livermore National Laboratory, for the first time, developed a Fast Adaptive Composite algorithm through a stand alone linear solver library, eliminating the need for users to "roll their own," as is the case presently. As a bonus, this interface also provides access to standard matrix-based solvers such as Incomplete Factorizations (ILU), Sparse Approximate Inverse methods, and Algebraic Multigrid (AMG), without requiring user code changes.

- *Pushing Collaboration beyond the Desktop.* Researchers at the Argonne National Laboratory continue to push technology to enable scientific collaborations with the Access Grid. The Access Grid is the ensemble of resources that can be used to support group-to-group human interaction across the grid. It consists of multimedia display, presentation and interactions environments, interfaces to grid middleware, and interfaces to visualization environments; and it supports large-scale distributed meetings, collaborative work sessions, seminars, lectures, tutorials and training. More than fifty Access Grid "nodes" -- including cameras, microphones and speakers, and multiple computers for audio and video -- have been installed worldwide.

- Novel Computer Interface and Visualization Environment Transferred to Industry. The 3D human-computer interface and visualization environment known as FLIGHT developed by researchers at the Sandia National Laboratories has been commercialized by Novint Technologies. This software represents several "firsts:"

  - First effort to integrate the sense of touch, with real-time graphics interaction.
  - First human interface totally based on 3D interaction tools. Three patents have been submitted.
  - First Trans-Atlantic virtual collaborative environment to interact with force feedback immersively. This work was presented as an invited application at the $2^{nd}$ International Grid booth at INET'2000.

- *A Lucky Catch: The Oldest, Most Distant Type Ia Supernova Confirmed by Supercomputer Analysis at NERSC.* An exploding star dubbed SN 1997ff, caught once on purpose and twice by accident by NASA's Hubble Space Telescope, is the oldest and most distant Type Ia supernova ever seen, according to a recent analysis performed at the Department of Energy's National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory. Scientists from the Lawrence Berkeley National Laboratory and the Space Telescope Science Institute that studied the distant supernova, used an IBM SP supercomputer to perform the analysis at NERSC, a world-class, 5 Teraflop, unclassified supercomputing center. By digitally subtracting images from the same region of space taken on two different dates, the researchers were able to isolate a supernova event and unravel much of the uncertainty associated with the observed data. As a result of their simulations, these researchers determined that the supernova was of Type Ia at a redshift of 1.7, and was first observed eight days after it exploded.

- *Fast Visualization of Vector Fields Using Color Mapping.* Researchers at the Sandia National Laboratory have developed two new techniques for visualizing two-dimensional vector fields that use color mapping to depict the flow direction. These approaches are fast because unlike conventional flow visualization techniques such as streamlines, they are completely local and require very little computation. This is especially significant for very large data sets where detection of small complex features is desired in real time. These approaches use the viewer's inherent ability to recognize and understand complex color patterns.
- *Twelve Companies Adopt Argonne Lab/USC Globus ToolkitTM as Standard Grid Technology Platform.* The open source Globus Toolkit$^{TM}$ developed by USC's Information Sciences Institute (ISI) and Argonne National Laboratory has become the de-facto international standard in the burgeoning field of grid computing as twelve leading computer vendors and software providers in the U.S. and Japan announced in November 2001, that they will port and/or support the product. Grid computing is a technology that uses the Internet as basic wiring to let people share computing, storage, data, programs, and other resources, just like the electric power grid allows people and energy companies to share generators of all kinds. The goal is to allow anyone with a computer to effectively integrate instruments, displays, and computational and information resources over a variety of computer platforms.
- *NERSC completes acquisition of new supercomputer.* The Department of Energy's National Energy Research Scientific Computing (NERSC) Center at Lawrence Berkeley National Laboratory has accepted and placed into full service its NERSC-3/Phase 2 system. In June 2001, this 5 Teraflop supercomputer system was number two on the "Top 500" list of the most powerful supercomputers in the world. The system meets, or exceeds, all major, original performance specifications. In FY 2002, its first full year of operation, NERSC-3 will provide the DOE Office of Science research community with 45,000,000 massively parallel processing (MPP) hours for simulations, which is almost a factor of two times the computational capability of the Center one year ago.

## AWARDS

### Mathematical, Information and Computational Sciences

- *R&D 100 Award*. An R&D 100 award was made to the to the University of Tennessee and Oak Ridge National Laboratory for developing the Performance Application Programming Interface (PAPI). PAPI specifies an application programming interface for accessing hardware performance counters available on most modern microprocessors. PAPI exploits these hardware counters to provide users with precise, high-resolution information on the number and timing of operations performed during software execution, on accesses to the memory hierarchy, on the status of instruction pipelines, and on all the aspects of software execution that must be analyzed when tuning software for high performance.

- *NERSC User Honored by American Physical Society Award for Work in Computational Physics.* Alex Zunger, a physicist at DOE's National Renewable Energy Laboratory in Colorado and a NERSC user, has been named the 2001 recipient of the prestigious Rahman Award by the American Physical Society. The award is presented annually to an individual for "outstanding achievement in computational physics research." Zunger was cited for his "pioneering work on the computational basis for first-principles electronic theory of solids." The Institute for Scientific Information has listed Zunger as one of the most-cited physicists worldwide.
- *Electronic Notebook Recognized for Innovation.* The Electronic Notebook software, enote v1.10, developed by the Oak Ridge National Laboratory and first released in 1999 received an Energy 100 Award in January 2001. These awards recognized the top 100 discoveries and innovations from the Department of Energy that have resulted in improvements for American consumers between 1973 and 2000. Enote provides an easy to use electronic lab notebook that has the look and feel of a scientist's paper notebook, but with additional digital features.

**Laboratory Technology Research**

- *R&D 100 Award - A New Catalyst Material to Treat Vehicle Exhaust Emissions.* Pacific Northwest National Laboratory (PNNL), in collaboration with Delphi Automotive Systems and Ford Research Laboratory, has developed a zeolite-Y-based-catalyst material for plasma-catalysis engine exhaust treatment that has been shown to remove nearly 90% of Nox, with a cost to fuel efficiency of less than 5%. Unlike other possible catalytic systems, this system is not harmed by sulfur impurities and requires no major design changes to vehicles or fuel infrastructure.
- *Federal Laboratory Consortium (FLC) Award for Excellence in Technology Transfer - Development of High-Temperature Superconducting Wires.* Oak Ridge National Laboratory (ORNL), in collaboration with Minnesota Mining and Manufacturing (3M), has developed a new route to the fabrication of high-temperature superconducting (HTS) wires for high power applications. These HTS materials have tremendous potential for greatly improved energy efficiency in a number of power applications related to the utilization of electrical energy. For example, these materials should produce superconducting transmission lines capable of 2-5 times the power transfer into urban areas, without need for additional rights-of-way and without significant losses to resistance.
- The 2001 Thomas Young Medal and Prize from the Instititute of Physics to a group leader in the Solid State Division of ORNL (awarded in 2001).

PROGRAM SHIFTS

In FY 2003, the MICS subprogram of ASCR will continue its components of the collaborative program across the Office of Science to produce the scientific computing, networking and collaboration tools that DOE researchers will require to address the scientific challenges of the next decade. This program was described in the March 2000 report to Congress entitled, "Scientific Discovery through Advanced Computing," (SciDAC). These activities build on the historic strength of the Department of Energy's Office of Science in computational science, computer science, applied mathematics, and high-performance computing and in the design, development, and management of large scientific and engineering projects and scientific user facilities.

In FY 2003, ASCR will enhance its investments in Advanced Computing Research Testbeds to provide additional specialized capabilities to SciDAC applications research teams that demonstrate significant opportunities for new scientific discovery. The partnership with the Biological and Environmental Research program initiated in FY 2001 in the areas of advanced mathematical, modeling and simulation techniques for biological systems will be expanded. New research will be undertaken to characterize the inventory of multiprotein molecular machines found in a subset of DOE-relevant microbes and organisms with nucleated cells (eukaryotes) and to simulate functional diversity. Results from these investigations are expected to impact clean energy, environmental cleanup, and carbon sequestration efforts. ASCR's contributions to this partnership will consist of developing the underlying mathematical understanding and computational tools that are needed for the analysis and simulation of these biological processes. Finally, in FY 2003, ASCR will initiate a new partnership with the Basic Energy Sciences program in the area of computational nanoscale science, engineering and technology. This partnership is an integral part of the Nanoscale Science, Engineering and Technology initiative in the Office of Science that is led by the Basic Energy Sciences program. The first goal of this initiative is to establish a fundamental scientific understanding of structures and interactions at the nanoscale. For example, it is known that when sample size, grain size, or domain size shrink to the nanoscale, collective phenomena can have a significant influence on local physical properties and may differ dramatically from the corresponding properties in bulk material. The principal missions of the Department of Energy (DOE) in science, energy, defense, and environment will benefit greatly from developments in these areas. Nanoscale synthesis and assembly methods will result in significant improvements in solar energy conversion; more energy-efficient lighting; stronger, lighter materials that will improve efficiency in transportation; greatly improved chemical and biological sensing; use of low-energy chemical pathways to break down toxic substances for environmental remediation and restoration; and better sensors and controls to increase efficiency in manufacturing. ASCR's contributions to this partnership will consist of developing the specialized computational tools for nanoscale science.

A Federally-chartered advisory committee was established for the Advanced Scientific Computing Research program in FY 2000 and 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. This advisory committee will play a key role in evaluating future planning efforts for research and facilities.

### *Interagency Environment*

The research and development activities supported 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 represents the evolution of 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 a key participant in these coordination bodies from the outset and will continue to coordinate its R&D efforts closely through this process.

In FY 1999, the President's Information Technology Advisory Committee (PITAC) recommended significant increases in support of basic research in: Software; Scalable Information Infrastructure; High End Computing; Socio-Economic and Workforce Impacts; support of research projects of broader scope; and visionary "Expeditions to the 21st Century" to explore new ways that computing could benefit our world.

Although the focus of the enhanced DOE program is on solving mission critical problems in scientific computing, this program will make significant contributions to the Nation's Information Technology Basic Research effort just as previous DOE mission-related research efforts have led to DOE's leadership in this field. In particular, the MICS subprogram will place emphasis on software research to improve the performance of high-end computing as well as research on the human-computer interface and on information management and analysis techniques needed to enable scientists to manage, analyze and visualize data from their simulations, and develop effective collaboratories. DOE's program, which focuses on the information technology research needed to enable scientists to solve problems in their disciplines, differs from the National Science Foundation's portfolio, which covers all of information technology. In addition, DOE's focus on large teams with responsibility for delivering software that other researchers can rely on differs from NSF's single investigator focus.

## Scientific Facilities Utilization

The ASCR program request includes $28,244,000 in FY 2003 to support the National Energy Research Scientific Computing (NERSC) Center, which is ASCR's component of the SC-wide Scientific Facilities Initiative that started in FY 1996. This investment will provide computer resources for about 2,400 scientists in universities, federal agencies, and U.S. companies. It will also leverage both federally and privately sponsored research, consistent with the Administration's strategy for enhancing the U.S. National science investment. The proposed funding will enable NERSC to maintain its role as one of the Nation's premier unclassified computing centers, which is a critical element in the success of many SC research programs. Research communities that benefit from NERSC include structural biology; superconductor technology; medical research and technology development; materials, chemical, and plasma sciences; high energy and nuclear physics; and environmental and atmospheric research.

## 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 2003, 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.

## Funding Profile

(dollars in thousands)

| | FY 2001 Comparable Appropriation | FY 2002 Original Appropriation | FY 2002 Adjustments | FY 2002 Comparable Current Appropriation | FY 2003 Request |
|---|---|---|---|---|---|
| Advanced Scientific Computing Research | | | | | |
| Mathematical, Information, and Computational Sciences | 151,647 | 155,050 | -650 | 154,400 | 166,625 |
| Laboratory Technology Research | 9,649 | 3,000 | 0 | 3,000 | 3,000 |
| Subtotal, Advanced Scientific Computing Research | 161,296 | 158,050 | -650 | 157,400 | 169,625 |
| General Reduction | 0 | -650 | 650 | 0 | 0 |
| Total, Advanced Scientific Computing Research | 161,296 [a] [b] | 157,400 | 0 | 157,400 | 169,625 |

**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 $3,990,000 which was transferred to the SBIR program and $239,000 which was transferred to the STTR program.

[b] Excludes $225,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

## Funding by Site

| | (dollars in thousands) | | | | |
|---|---|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 | $ Change | % Change |
| Albuquerque Operations Office | | | | | |
| Los Alamos National Laboratory | 5,727 | 2,855 | 5,020 | +2,165 | +75.8% |
| Sandia National Laboratories | 4,656 | 4,767 | 3,889 | -878 | -18.4% |
| Total, Albuquerque Operations Office | 10,383 | 7,622 | 8,909 | +1,287 | +16.9% |
| Chicago Operations Office | | | | | |
| Ames Laboratory | 2,151 | 1,991 | 1,625 | -366 | -18.4% |
| Argonne National Laboratory | 14,077 | 11,246 | 8,573 | -2,673 | -23.8% |
| Brookhaven National Laboratory | 2,130 | 1,199 | 542 | -657 | -54.8% |
| Fermi National Accelerator Laboratory | 120 | 226 | 60 | -166 | -73.5% |
| Princeton Plasma Physics Laboratory | 190 | 340 | 0 | -340 | -- |
| Chicago Operations Office | 28,161 | 12,060 | 7,240 | -4,820 | -40.0% |
| Total, Chicago Operations Office | 46,829 | 27,062 | 18,040 | -9,022 | -33.3% |
| Oakland Operations Office | | | | | |
| Lawrence Berkeley National Laboratory | 65,807 | 51,325 | 53,223 | +1,898 | +3.7% |
| Lawrence Livermore National Laboratory | 4,898 | 6,587 | 3,068 | -3,519 | -53.4% |
| Stanford Linear Accelerator Center | 315 | 502 | 234 | -268 | -53.4% |
| Oakland Operations Office | 4,316 | 1,781 | 960 | -821 | -46.1% |
| Total, Oakland Operations Office | 75,336 | 60,195 | 57,485 | -2,710 | -4.5% |
| Oak Ridge Operations Office | | | | | |
| Oak Ridge Inst. For Science and Education | 349 | 100 | 99 | -1 | -1.0% |
| Oak Ridge National Laboratory | 22,545 | 11,251 | 10,496 | -755 | -6.7% |
| Thomas Jefferson National Accelerator Facility | 50 | 0 | 0 | 0 | -- |
| Oak Ridge Operations Office | 60 | 0 | 0 | 0 | -- |
| Total, Oak Ridge Operations Office | 23,004 | 11,351 | 10,595 | -756 | -6.7% |
| Richland Operations Office | | | | | |
| Pacific Northwest National Laboratory | 4,616 | 3,738 | 1,003 | -2,735 | -73.2% |
| Washington Headquarters | 1,128 | 47,432 | 73,593 | +26,161 | +55.2% |
| Total, Advanced Scientific Computing Research | 161,296 [a] [b] | 157,400 | 169,625 | +12,225 | +7.8% |

[a] Excludes $3,990,000 which was transferred to the SBIR program and $239,000 which was transferred to the STTR program.

[b] Excludes $225,000 which was transferred to the Science Safeguards and Security program in an FY 2001 reprogramming.

# 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 testbed at ANL focuses on a large cluster of Intel-based compute nodes with an open source operating system based on LINUX, this cluster has been given the name of "Chiba City." 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. 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 significant participation in the advanced computing software tools program as well as basic research in applied mathematics and participates on a number of the SciDAC teams.

## 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 collaboratory 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 collaboratory tools. ORNL also participates in several scientific application and collaboratory 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 from Compaq and IBM including significant interactions with SciDAC applications teams. 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 collaboratory 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 collaboratory tools. SNL also participates in several scientific application and collaboratory 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 117 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 Objectives

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.

- A key feature of the ASCR program is that the approach to accomplishing the Program Strategic Performance Goals is integrated through the management of the MICS subprogram. Computing and networking requirements of the Office of Science far exceed the current state-of-the-art; and the requirements far exceed the tools that the commercial marketplace will deliver. The MICS subprogram must not only support basic research in the areas listed above, but also the development of the results from this basic research into software usable by scientists in other disciplines and partnerships with users to test the usefulness of the research. These partnerships with the scientific disciplines are critical because they provide rigorous tests of the usefulness of current advanced computing research, enable MICS to transfer the results of this research to scientists in the disciplines, and help define promising areas for future research. This integrated approach is critical for MICS to succeed in providing the extraordinary computational and communications tools that DOE's civilian programs need to carry out their missions. It is important to note that these tools have applications beyond the Office of Science; to the NNSA and the private sector after these tools have been initially discovered and developed by the MICS subprogram.

In addition to its research activities, the MICS subprogram supports the operation of 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.

In FY 2003, the MICS subprogram will continue its components of the collaborative SciDAC program across the Office of Science to produce the scientific computing, networking and collaboration tools that DOE researchers will require to address the scientific challenges of the next decade. The MICS components include investments in scientific computing research and networking and collaboration research that are complemented by investments in computing and networking facilities. In addition, in FY 2003, MICS will increase its efforts in computational biology and in computational nanoscience.

The specific details of the MICS investment strategy are described below in the detailed program justification section of this budget. However, it is important to understand that all of those individual program elements are pieces in a puzzle whose overall goal is to enable scientists to use computing and collaboration technologies as tools for scientific discovery. Thus, the way the individual elements fit together and complement each other is critical because a scientist needs all of these pieces to succeed. A weakness in any one element, or weakness in the way the elements are integrated, are barriers to the scientist's success. The three sections below provide the background for MICS subprogram investments in Scientific Computing Research, High Performance Networking, Middleware and Collaboratory Research, and High Performance Computing and Networking Facilities.

## Scientific Computing Research Investments

In scientific computing, the key measure of success in translating peak computing power into science is the percent of peak performance that is delivered to an application over the *entire* calculation. In the early to mid-1990's on computers such as the Cray Research C-90, many scientific codes realized 40% to 50% of the peak performance of the supercomputer. In contrast, on today's parallel supercomputers, scientific computing codes often realize only 5% to 10% of "peak" performance, and this fraction could decrease as the number of processors in the computers grow.

This phenomenon is a direct result of the fact that the speed of memory systems and the speed of interconnects between processors is increasing much more slowly than processor speed. For many scientific applications these factors dominate the performance of the application. Two types of solutions are available to the computer hardware designer in addressing the mismatch of speed between the components: (1) clever hierarchical arrangements of memory with varying speeds and software to find data before it is needed and move it into faster memory, closer to the processor that will need it; and (2) techniques to increase parallelism, for example, by using threads in the processor workloads or by combining parallel data streams from memory or disks. Current technology forecasts indicate a doubling or quadrupling in the numbers of layers in the memory hierarchy, and a 100- to 1000-fold increase in the amount of parallelism in disk and tape systems to accommodate the relative increase in the mismatch between processor speed and memory, disk and tape speeds in the next five years.

One result of this increasing complexity of high-performance computer systems is the importance of the underlying systems software. Operating systems, compilers, runtime environments, mathematical libraries, and end-user applications must all work together efficiently to extract the desired high performance from these systems.

In addition to the challenges inherent to managing the required level of parallelism, technology trends and business forces in the U.S. computer system industry have resulted in radically reduced development and production of high-end systems necessary for meeting the most demanding requirements of scientific research. In essence, the U.S. computer industry has become focused on the computer hardware and software needs of business applications, and little attention is paid to the special computational needs of the scientific community. Therefore, to achieve the performance levels required for agency missions and world leadership in computational science, large numbers of smaller commercial systems must be combined and integrated to produce terascale computers. Unfortunately, the operating systems software and tools required for effective use of these large systems are significantly different from the technology offered for the individual smaller components. Therefore, new enabling software must be developed if scientists are to take advantage of these new computers in the next five years.

The following are specific examples of *computer science* research challenges:

- 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.

In addition to these computer science challenges, significant enhancements to the MICS applied mathematical research activity are required for the Department to satisfy its mission requirements for computational science. Over the history of computing, improvements in algorithms have yielded at least as much increase in performance as has hardware speedup. Large proportions of these advances are the products of the MICS applied mathematics research activity. In addition to improving the speed of the calculations, many of these advances have dramatically increased the amount of scientific understanding produced by each computer operation. For example, a class of mathematical algorithms called "fast multipole algorithms," was discovered for a number of important mathematical operations required to process 1,000 datapoints by a factor of 1,000; 10,000 datapoints by a factor of 10,000; and so on. Another example of how powerful these methods can be is that they enable a scientist to process 10,000 datapoints in the time that it would have taken to process 100 using earlier techniques, or 1,000,000 datapoints in the time older techniques would have needed to process 1,000. 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 domain scientists. In this area of research the MICS applied mathematics activity is the core of the nationwide effort.

The MICS subprogram will address these challenges by continuing the competitively selected partnerships (based on solicitation notices to DOE national laboratories and universities) focused on discovering, developing, and deploying to scientists key enabling technologies that were initiated in FY 2001. These partnerships, which are called Integrated Software Infrastructure Centers, must support the full range of activities from basic research through deployment and training because the commercial market for software to support terascale scientific computers is too small to be interesting to commercial software providers. These centers play a critical role in providing the software infrastructure that will be used by the SciDAC applications research teams. The management of these centers will build on the successful experience of the MICS subprogram in managing other community software research efforts as a part of its High Performance Computing and Communications program, as well as on the lessons learned in important programs supported by Defense Advanced Research Projects Agency (DARPA) such as Project Athena at MIT, the Berkeley UNIX Project, and the initial development of the Internet software and the Internet Activities Board (IAB). These Integrated Software Infrastructure Centers will have close ties to key scientific applications projects to ensure their success.

The efforts initiated in FY 2001 address the important issues of understanding and developing the tools that applications developers need to make effective use of machines that will be available in the next several years.

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

- Applied Mathematics,
- Computer Science, and
- 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 the solution of complex problems. It is now becoming possible to effectively harness and integrate the collective capabilities of large geographically distributed computational facilities, data archives, and research teams. This new 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.

- Significant research is needed to augment the capability and performance of today's networks, including the Internet, in order to develop high-performance network infrastructures that support distributed high-end data-intensive applications and secure large-scale scientific collaboration. 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, and traffic models of large single flows.
- 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. These high-performance middleware provide the scalable software components needed to integrated distributed data archives, high performance disk caches, visualization and data analysis servers, authentication and security services, computational resources, and the underlying high-speed network networks into a scalable and secure scientific collaborative environment.

The MICS subprogram will address these challenges through an integrated program of fundamental research in networking and 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, and
- 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 and other leading-edge instruments and facilities.
- **Advanced Computing Research Testbeds.** These testbeds provide advanced computational hardware for testing and evaluating new computing hardware and software. These testbeds are providing specialized computational resources to support SciDAC applications teams in FY 2002. In FY 2003, this activity will be enhanced to provide specialized computing resources to SciDAC application teams.

Current production supercomputing resources provided less than half of the resources that were requested last year. The pressure on production facilities will only increase in future years as more applications become ready to move from testing the software to using the software to generate new science. In addition, as the speed of computers increases, the amount of data they produce also increases. 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. These network enhancements are also required to allow researchers to have effective remote access to the experimental facilities that the Office of Science provides for the Nation.

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, and
- Energy Sciences Network (ESnet).

## Funding Schedule

(dollars in thousands)

| | FY 2001 | FY 2002 | FY 2003 | $ Change | % Change |
|---|---|---|---|---|---|
| Mathematical, Computational, and Computer Sciences Research | 57,434 | 70,315 | 78,620 | +8,305 | +11.8% |
| Advanced Computation, Communications Research and Associated Activities | 94,213 | 80,139 | 83,782 | +3,643 | +4.5% |
| SBIR/STTR | 0 | 3,946 | 4,223 | +277 | +7.0% |
| Total, Mathematical, Information, and Computational Sciences | 151,647 | 154,400 | 166,625 | +12,225 | +7.9% |

## Detailed Program Justification

(dollars in thousands)

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| **Mathematical, Computational, and Computer Sciences Research** | **57,434** | **70,315** | **78,620** |
| ■ **Applied Mathematics** | **27,110** | **32,000** | **24,634** |

Research is conducted on the underlying mathematical understanding and numerical algorithms to enable effective description and prediction of physical systems. Research in applied mathematics is critical to the DOE's mission because improved mathematical techniques enable large computational simulations. As discussed earlier in the MICS subprogram overview, improvements in mathematical algorithms are responsible for greater improvement in scientific computing capabilities than the increases in hardware performance. This activity supports research at DOE laboratories, universities, and private companies at a level similar to previous years. Many of the projects supported by this activity are partnerships among researchers at universities and DOE laboratories. The program supports research in a number of areas including: ordinary and partial differential equations, including numerical linear algebra, iterative methods and preconditioners, sparse solvers, and dense solvers; fluid dynamics, including compressible, incompressible and reacting flows, turbulence modeling, and multiphase flows; optimization, including linear and nonlinear programming, interior-point methods, and discrete and integer programming; mathematical physics; control theory, including differential-algebraic systems, order reduction, queuing theory; shock wave theory systems, multipole expansions, mixed elliptic-hyperbolic problems, including hyperbolic and wavelet transforms; dynamical systems, including chaos-theory and control, and bifurcation theory; programming; and geometric and symbolic computing, including minimal surfaces and automated reasoning systems.

The FY 2003 budget continues the FY 2001 increased level of funding for the Computational Sciences Graduate Fellowship program. In addition, the FY 2003 budget includes a $2,000,000 increase to support basic research in applied mathematics focused on developing the mathematical understanding and techniques needed for our partnership with the Biological and Environmental

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |

Research program. This partnership focuses on understanding microbes that address DOE energy and environmental needs through a research program on the leading edge of biology. The research will offer new ways to solve environmental challenges related to DOE's missions, including toxic waste cleanup, new clean energy sources and global climate stabilization through carbon sequestration. New research in applied mathematics is needed to support this partnership because the needs of biologists include areas of mathematical research such as graph theory, combinatorics, control theory, and advanced statistics research that are not supported by the existing program.

FY 2003 funding for the competitively selected Integrated Software Infrastructure Centers (ISICs) partnerships focused on algorithms and mathematical libraries for critical DOE applications on terascale computers, which had previously been under this activity, has been transferred to the Advanced Computing Software Tools activity, along with the FY 2003 funding for the ISICs that had previously been under the Computer Science activity. This transfer enables a clearer discussion of these activities and a clearer relationship to the ASCR Program Strategic Performance Goals.

**Performance will be measured** in a number of ways. Efforts in applied mathematics will be evaluated on an ongoing basis for their leadership and significant contributions to the worldwide applied mathematics effort using measures including a number of awards, significant advances, and invited participation and membership on organizing and program committees of major national and international conferences (SC5-1; SC5-2). The Computational Science Graduate Fellowship Program will appoint 20 new students to develop the next generation of leaders in computational science for DOE and the Nation (SC5-1).

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| ■ **Computer Science**................................................................ | **20,941** | **21,051** | **19,000** |

Research in computer science to enable large scientific applications is critical to DOE because its unique requirements for high performance computing significantly exceed the capabilities of computer vendors' standard products. Therefore, much of the computer science to support this scale of computation must be developed by DOE. This activity supports 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, carry out this research.

FY 2003 funding for the competitively selected Integrated Software Infrastructure Centers (ISICs) partnerships focused on computer science research for critical DOE applications on terascale computers, which had previously been under this activity, has been transferred to the Advanced Computing Software Tools activity, along with the FY 2003 funding for the ISICs that had previously been under the Applied Mathematics activity. This transfer enables a clearer discussion

| | (dollars in thousands) | |
|---|---|---|
| FY 2001 | FY 2002 | FY 2003 |

of these activities and a clearer relationship to the ASCR Program Strategic Performance Goals.

**Performance in computer science will be measured** through peer review and regularly scheduled external expert reviews of ongoing projects, production of significant research results, and the adaptation of results and knowledge by other researchers supported by the Office of Science (SC5-1; SC5-2).

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| ■ **Advanced Computing Software Tools** ................................ | **4,421** | **8,473** | **20,256** |

This research uses the results of fundamental research in applied mathematics and computer science to develop an integrated set of software tools that scientists in various disciplines can use to develop high performance applications (such as simulating the behavior of materials). These tools, that provide 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 2003, support for all the competitively selected Integrated Software Infrastructure Centers, competitively selected in FY 2001 under SciDAC, to address critical computer science and systems software issues for terascale computers is described in this activity for clarity. FY 2003 funding for basic research in computer science focused on problem solving environments for scientific computing, portable runtime systems, and other basic research in software components, which was previously included in this activity has been transferred to the computer science activity in order to more clearly characterize the research.

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 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 strategy for SciDAC. The ISICs differ from the other activities in this program element because they are responsible for the entire lifecycle of the software that they develop. From the experience gained with end user application scientists applying previous software tools, it has become clear that to promote wide usage across the scientific community, the tools must also be reliable, documented, and easy to use. In addition, users of the tools need the tools to be maintained so that the tools continue to be available, have bugs fixed, etc. Since many of the tools needed in the high performance arena have no commercial market, the Integrated Software Infrastructure Centers initiated in FY 2001 will provide a means for focused investment to deploy these tools to the scientific community.

**Performance will be measured** through peer review and regularly scheduled external expert reviews of ongoing projects, production of significant research results, and the adaptation of results and knowledge by other researchers in the Office of Science (SC5-1; SC5-2). In addition, these ISICs will undergo a progress review to ensure effective coupling between the ISICs and between the ISICs and application teams in the MICS Scientific Applications Pilot Projects efforts and in the SciDAC teams funded by the other programs in the Office of Science (SC5-2).

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| ■ **Scientific Applications Pilot Projects**.................................. | **4,962** | **8,791** | **14,730** |

This research is a collaborative effort with disciplinary computational scientists to apply the computational techniques and tools developed by MICS supported research to basic research problems relevant to the mission of SC. This effort tests the usefulness of current advanced computing research, transfers the results of this research to the scientific disciplines, and helps define promising areas for future research. The FY 2003 funding for this activity will allow the continuation of the pilot projects that were competitively selected in FY 2001. These pilot projects are tightly coupled to the Integrated Software Infrastructure Centers (described above in advanced computing software tools) to ensure that these activities are an integrated approach to the challenges of terascale simulation and modeling that DOE faces to accomplish its missions. These partnerships include areas such as design of particle accelerators with the High Energy and Nuclear Physics (HENP) program; 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 increase in funding in this program activity will focus on expanding our partnership with BER and establishing a new partnership with BES. This expansion of the partnership with BER includes an increase of approximately $3,000,000 in FY 2003, which further develops the computational research infrastructure needed to study microbial communities that may have applications to clean energy, environmental cleanup, and carbon sequestration and especially underlying mathematical understanding and computational tools that are needed for the analysis and simulation of these biological processes. The new partnership with the BES program includes approximately $3,000,000 for computational nanoscale science engineering and technology. This partnership is an integral part of the Nanoscale Science, Engineering and Technology initiative in the Office of Science, that is led by the BES program. These new research teams will focus on using high performance computers to answer fundamental questions such as the emergence of collective phenomena -- phenomena that emerge from the interactions of the components of the material and whose behavior thus differs significantly from the behavior of those individual components. In some cases, collective phenomena can bring about a large response to a small stimulus -- as seen with colossal magnetoresistance, the basis of a new generation of recording memory material. Collective phenomena are also at the core of the mysteries of such materials as the high-temperature superconductors, one of the great outstanding problems in condensed matter physics. All of these new projects will be selected through open, peer reviewed competitive processes.

| | | (dollars in thousands) | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |

**Performance will be measured** through peer review, external expert reviews of ongoing projects, production of significant research results, and the adaptation of results and knowledge by other researchers supported by the Office of Science (SC5-2).

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| **Advanced Computation, Communications Research, and Associated Activities** | **94,213** | **80,139** | **83,782** |
| ■ **Networking** | **7,507** | **7,066** | **7,066** |

Research is needed to develop high-performance networks that are capable of supporting distributed high-end computing and secure large-scale scientific collaboration. High performance networks enable scientists to collaborate effectively and to have efficient access to distributed computing resources such as tera-scale computers, experimental scientific instruments, and large scientific data archives. This research is carried out at national laboratories and universities. It focuses in areas such as high-performance transport protocols for high-speed networks; scalable techniques for measuring, analyzing, and controlling traffic in high performance networks; network security research to support large-scale scientific collaboration; advanced network components to enable high-speed connections between terascale computers, large scientific data archives, and high-speed networks; and research on high-performance "middleware." Middleware is a collection of network-aware software components that scientific applications need in order to couple efficiently to advanced network services and make effective use of experimental devices, data archives, and terascale computers at different locations. In all of these cases, the network and middleware requirements of DOE significantly exceed those of the commercial market.

**Performance will be measured** through peer review, external expert reviews of ongoing projects, production of significant research results, and the adaptation of results and knowledge by other researchers supported by the Office of Science and other Federal Agencies (SC5-1; SC5-2).

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| ■ **Collaboratory Tools** | **5,915** | **5,527** | **5,527** |

This research uses the 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 across 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

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |

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. Finally, another example of research in collaboratory tools is the development of a scientific annotation middleware system that will provide significant advances in research documentation and data pedigree tracking. Researchers access the system through a notebook interface as well as through components embedded in other software systems. It will provide more complete, effective and efficient ways to document scientific work.

**Performance will be measured** through peer review, and regularly scheduled external expert reviews of ongoing projects, production of significant research results, and the adaptation of results by other researchers supported by the Office of Science and other Federal Agencies (SC5-2).

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| ■ **National Collaboratory Pilot Projects** ................................ | **8,245** | **10,857** | **10,857** |

This program is intended to test, validate, and apply 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 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 and Nuclear Physics (HENP) 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 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 badly 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

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |

distributed computation. This level of funding will permit the continuation of the efforts funded in FY 2001.

**Performance will be measured** through peer review, and regularly scheduled external expert reviews of ongoing projects, production of significant research results, and the adaptation of results by other researchers supported by the Office of Science (SC5-2).

| | | | |
|---|---|---|---|
| ■ **National Energy Research Scientific Computing Center (NERSC)** ........................................................................ | **34,361** | **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; 36 percent of users are university based, 59 percent are in National Laboratories, 4 percent are in industry, and 1 percent in other government laboratories. NERSC provides a spectrum of supercomputers offering a range of high performance computing resources and associated software support. The two major computational resources at NERSC are a 512 processor Cray T3E computer and a 2,944 processor IBM SP computer whose installation was completed in late FY 2001 following a fully competitive procurement process. The FY 2003 funding will support the operation of the IBM-SP computer at about 5.0 teraflops "peak" performance. These computational resources will be 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 2003 capital equipment requirements continue at the same level as in FY 2002. The competitive process for upgrading hardware (NERSC-4) is underway. The target date for the installation of NERSC-4 Phase I hardware is mid FY 2003. Expected performance will be greater than 10 teraflops.

**Performance will be measured** in a number of ways. Hardware performance is determined by computing the percentage of time the machine is actually available to users, which excludes scheduled downtime for maintenance, etc. This will be 90 percent or more of the total scheduled operating time. In FY 2001, the measured operating time lost to unscheduled downtime on systems at NERSC ranged from 0 percent to 1.34 percent. Overall performance of the center is measured by user surveys that will continue to show a high degree of satisfaction with the services at NERSC and annual reports that will continue to demonstrate production of world-class science being done at the facility. NERSC will be operated within budget while meeting user needs and satisfying overall SC program requirements (SC5-2; SC7-5)

| | | | |
|---|---|---|---|
| ■ **Advanced Computing Research Testbeds (ACRTs)**........... | **20,057** | **11,657** | **15,300** |

This activity supports the advanced computational hardware testbeds that play a critical role in testing and evaluating new computing hardware and software, especially with regard to their applicability to scientific problems. Current testbeds are located at Argonne National Laboratory (IBM/ Intel Cluster); and ORNL (Compaq-Alpha technology and IBM Power –4 technology). These testbeds represent the evolution of Advanced Computing Research Facilities that supported the computational requirements of the scientific application partnerships that were completed in

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |

FY 2000. Support for the Nirvana Blue Computer Testbed at LANL was phased out in FY 2001. This activity also supports the distributed high performance storage system (HPSS) testbed collaboration between ORNL and LBNL. Because many of the issues to be investigated only appear in the computer systems at significantly larger scale than the computer manufacturers' commercial design point, these testbeds must procure the largest scale systems that can be afforded and develop software to manage and make them useful. In addition, the ACRTs, taken together, must have a full range of computer architectures to enable comparison and reduce overall program risk. These all involve significant research efforts, often in partnership with the vendors to resolve issues including operating system stability and performance, system manageability and scheduling, fault tolerance and recovery, and details of the interprocessor communications network. Therefore, these systems are managed as research programs and not as information technology investments. The additional funding in this program element will enhance the ability of these testbeds to provide specialized computational resources to support SciDAC applications teams in FY 2003.

**Performance will be measured by** the importance of the research that results from these testbeds as viewed by publications in the scientific literature, the ASCR Advisory Committee and external reviews and the demand for access to these facilities by the nationwide computer and computational science communities (SC5-2; SC7-5)

| | FY 2001 | FY 2002 | FY 2003 |
|---|---|---|---|
| ■ **Energy Sciences Network (ESnet)** ...................................... | **18,128** | **16,788** | **16,788** |

ESnet is a high-performance network infrastructure that supplies the DOE science community with capabilities not available on current commercial networks or the commercial Internet. It provides national and international high-speed access to the DOE and to the Office of Science research facilities, including: advanced light sources; neutron sources; particle accelerators; fusion reactors; spectrometers; supercomputers; Advanced Computing Research Testbeds (ACRTs); and other leading-edge science instruments and facilities. ESnet provides the communications fabric that interconnects geographically distributed research facilities and large-scale scientific collaboration. It 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. For day-to-day operation, DOE employs ESnet management at LBNL, who contracts with commercial vendors for advanced communications services including Asynchronous Transfer Mode (ATM), Synchronous Optical Networks (SONET) and Dense Wave Division Multiplexing (DWDM). In addition, LBNL ESnet management is responsible for the 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. The FY 2003 funding will support the continued operation of ESnet and will meet capital equipment needs to upgrade high-speed network routers, ATM switches, and network testing equipment.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |
| **Performance will be measured** in several ways. The operating time lost due to unscheduled ESnet downtime in FY 2003 will be less than 10 percent of the total scheduled possible operating time. In FY 2001, the measured operating time lost to unscheduled downtime on ESnet was 3 percent of total scheduled operating time. In FY 2003, ESnet will operate within budget while meeting user needs and satisfying overall SC program requirements. Network enhancements will improve researchers access to high performance computing and software support, and enhance scientific opportunities by enabling scientists to access and understand greater amounts of scientific data and benefit DOE and scientific research (SC5-2; SC7-5). | | | |
| **SBIR/STTR** | **0** | **3,946** | **4,223** |
| In FY 2001, $3,748,000 and $225,000 were transferred to the SBIR and STTR programs, respectively. The FY 2002 and FY 2003 amounts are the estimated requirement for the continuation of the SBIR and STTR programs. | | | |
| **Total, Mathematical, Information, and Computational Sciences** | **151,647** | **154,400** | **166,625** |

## Explanation of Funding Changes from FY 2002 to FY 2003

| | FY 2003 vs. FY 2002 ($000) |
|---|---|
| **Mathematical, Computational, and Computer Sciences Research** | |
| ■ **Applied Mathematics.** Provides an increase to the Applied Mathematics program element to support research in applied mathematics for biological problems plus a small enhancement to the Computational Science Graduate Fellowship program ($2,366,000). The new research in applied mathematics will focus on the mathematics needed by biologists to understand microbes and include areas of mathematical research such as graph theory, combinatorics, control theory, and advanced statistics research. Funding for the ISICs previously included in the Applied Mathematics program element is transferred to the Advanced Computing Software Tools program element (-$9,732,000). This transfer more clearly identifies the special role of the ISICs and clarifies the budget description. | -7,366 |

| | FY 2003 vs. FY 2002 ($000) |
| --- | --- |
| ■ **Computer Science.** Transfers funding for the ISICs previously included in the Computer Science program element to the Advanced Computing Software Tools program element (-$7,051,000). Transfers funding for basic research in computer science focused on problem solving environments for scientific computing, portable runtime systems, and other basic research in software components, which was previously included in the Advanced Computing Software Tools program element to the Computer Science program element ($5,000,000). These transfers more clearly identify the special role of the ISICs and clarify the budget description................................................................................................................ | -2,051 |
| ■ **Advanced Computing Software Tools.** Transfers funding for the ISICs previously included in the Applied Mathematics ($9,732,000) and Computer Science ($7,051,000) program elements to the Advanced Computing Software Tools program element. Transfers funding for basic research in computer science focused on problem solving environments for scientific computing, portable runtime systems, and other basic research in software components, which was previously included the Advanced Computing Software Tools program element (-$5,000,000) to the Computer Science program element. These transfers more clearly identify the special role of the ISICs and clarifies the budget description.... | +11,783 |
| ■ **Scientific Application Pilot Projects.** Provides additional funding to double the number of pilot projects in the partnership with BER on computational biology, and to enable a number of new partnerships with BES focused on computational nanoscience. The new, competitively selected research teams in the partnership with BER will focus on the computational tools that are needed for the analysis and simulation of biological processes such as protein folding and gene regulation. The new, competitively selected research teams in the partnership with BES will focus on using high performance computers to answer fundamental questions in nanoscale science such as the emergence of collective phenomena............................ | +5,939 |
| **Advanced Computation, Communications Research, and Associated Activities** | |
| ■ **Advanced Computing Research Testbed.** Provides an increase in this program element to establish a minimal high-performance computing capability for Topical Applications, providing an architecture tailored to a class of applications within the SciDAC research portfolio to produce new science, including required upgrades to ESnet infrastructure.......................................................................... | +3,643 |
| **SBIR/STTR** | |
| ■ Increase in SBIR/STTR due to increase in operating expenses. ................................. | +277 |
| Total Funding Change, Mathematical, Information, and Computational Sciences ............. | +12,225 |

# Laboratory Technology Research

## Mission Supporting Goals and Objectives

The mission of the Laboratory Technology Research (LTR) 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. Therefore, the LTR subprogram is responsible for one of the ASCR Program Strategic Performance Goals:

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 2001 | FY 2002 | FY 2003 | $ Change | % Change |
| Laboratory Technology Research ........... | 9,649 | 2,921 | 2,921 | 0 | -- |
| SBIR/STTR ............................................ | 0 | 79 | 79 | 0 | -- |
| Total, Laboratory Technology Research.. | 9,649 | 3,000 | 3,000 | 0 | -- |

## Detailed Program Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2001 | FY 2002 | FY 2003 |
| **Laboratory Technology Research** | **9,649** | **2,921** | **2,921** |

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 hydroporphyrin 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.

**Performance in this activity will be measured** through merit-based peer and on-site reviews.

| | | | |
|---|---|---|---|
| **SBIR/STTR** | **0** | **79** | **79** |

In FY 2001, $242,000 and $14,000 were transferred to the SBIR and STTR programs, respectively. The FY 2002 and FY 2003 amounts are the estimated requirement for the continuation of the SBIR and STTR program.

| | | | |
|---|---|---|---|
| **Total, Laboratory Technology Research** | **9,649** | **3,000** | **3,000** |

## Explanation of Funding Changes from FY 2002 to FY 2003

| | FY 2003 vs. FY 2002 ($000) |
|---|---|
| There are no significant funding changes. | |

# Capital Operating Expenses & Construction Summary

## Capital Operating Expenses

(dollars in thousands)

| | FY 2001 | FY 2002 | FY 2003 | $ Change | % Change |
|---|---|---|---|---|---|
| General Plant Projects | 0 | 1,000 | 1,000 | 0 | -- |
| Capital Equipment (total) | 5,213 | 5,130 | 6,250 | +1,120 | +21.8% |
| Total, Capital Operating Expenses | 5,213 | 6,130 | 7,250 | +1,120 | +18.3% |

## Major Items of Equipment (TEC $2 million or greater)

(dollars in thousands)

| | Total Estimated Cost (TEC) | Prior Year Approp- riations | FY 2001 | FY 2002 | FY 2003 | Accept- ance Date |
|---|---|---|---|---|---|---|
| Distributed Visualization Server – LBNL | 2,500 | 0 | 2,500 | 0 | 0 | FY 2001 |
| Total, Major Items of Equipment | | 0 | 2,500 | 0 | 0 | |