Advanced Scientific Computing Research

Program Mission

The primary mission of the Advanced Scientific Computing Research (ASCR) program, which is carried out by the Mathematical, Information, and Computational Sciences subprogram, is to discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the Department of Energy. To accomplish this mission the program fosters and supports fundamental research in advanced scientific computing – applied mathematics, computer science, and networking – and operates supercomputer, networking, and related facilities. The applied mathematics research efforts provide the fundamental mathematical methods to model complex physical and biological systems. The computer science research efforts enable scientists to efficiently run these models on the highest performance computers available and to store, manage, analyze, and visualize the massive amounts of data that result. The networking research provides the techniques to link the data producers; e.g., supercomputers and large experimental facilities with scientists who need access to the data.

In fulfilling this primary mission the ASCR program supports the Office of Science Strategic Plan's goal of providing extraordinary tools for extraordinary science as well as building the foundation for the research in support of the other goals of the strategic plan. In the course of accomplishing this mission, the research programs of ASCR have played a critical role in the evolution of high performance computing and networks.

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

The high quality of the research in the entire ASCR program, supporting both of its missions, is continuously evaluated through the use of merit-based peer review and scientific advisory committees.

Program Goals

- Maintain world leadership in areas of advanced scientific computing research relevant to the missions of the Department of Energy.
- Integrate the results of advanced scientific computing research into the natural sciences and engineering.
- Provide world-class supercomputer and networking facilities for scientists working on problems that are important to the missions of the Department.
- Integrate and disseminate the results of high-risk research in natural sciences and engineering to the private sector through the Laboratory Technology Research subprogram.

Program Objectives

- *Advance the frontiers of knowledge in advanced scientific computing research.* – Foster research to create a new fundamental knowledge in areas of advanced computing research important to the Department, e.g., high performance computing, high speed networks to support scientific collaborations, and software to enable scientists to make effective use of the highest performance computers available.

- *Apply advanced computing knowledge to complex problems of importance to DOE.* — Promote the transfer of the results of advanced scientific computing research to DOE missions in areas such as the improved use of fossil fuels including understanding the combustion process; the atmospheric and environmental impacts of energy production and use including global climate modeling and subsurface transport; and future energy sources including fusion energy as well as the fundamental understanding of matter and energy.
- *Plan, construct, and operate premier supercomputer and networking facilities.* — Serve researchers at national laboratories, universities, and industry, thus enabling both new understanding through analysis, modeling, and simulation of complex problems and effective integration of geographically distributed teams through national collaboratories.
- *Transfer results of fundamental research to the private sector.* — Provide tangible results of research and development activities through cost-shared partnerships with industry.

Performance Measures

The Advanced Scientific Computing Research program measures performance in various ways, depending on the objective. However, performance measures fall into four broad categories:

- peer review, which is the key performance measurement process of all research activities;
- indicators or metrics (i.e., things that can be counted);
- customer evaluation and stakeholder input; and
- qualitative assessments, which might include historical retrospectives and annual program highlights.

Facility performance measures include achievement of performance specifications, operating time, throughput, user satisfaction, and effective utilization of resources as determined by reports from external review panels, user steering committees, and internal Office of Science (SC) program manager committees. In addition, ASCR supercomputer and network facilities have periodic external performance reviews. The Energy Sciences Network (ESnet) operations and management were reviewed in this manner in FY 1998.

Performance Measures for FY 2001 include:

- conduct regular peer review and merit evaluation based on the principles set down in 10 CFR Part 605 for grants and cooperative agreements, with all research projects reviewed at least once and no project extending more than four years without review;
- support the Computational Science Graduate Fellowship Program with the successful appointment of 10 new students to support the next generation of leaders in computational science for DOE and the Nation;
- the operating time lost at scientific facilities due to unscheduled NERSC/ESnet downtime will be less than 10 percent of the total scheduled possible operating time, on average;
- facilities, including the National Energy Research Scientific Computing Center (NERSC) and ESnet, will be operated within budget and successfully meet user needs and satisfy overall SC program requirements where, specifically, NERSC will deliver 3.6 Teraflop capability by the end of FY 2001 to support DOE's science mission;
- work performed by investigators supported by ASCR will continue to be recognized as outstanding through the receipt of major prizes and awards;
- the Laboratory Technology Research subprogram will complete its review of projects initiated during the previous year to ensure that research objectives and program goals are being met;

- research in predictability of computer simulations will provide a common intellectual foundation and a set of tools for evaluating predictability issues. These tools will be used by initiatives to use computational simulation across the Department, including climate research, combustion modeling, and stockpile stewardship.
- the Advanced Computing Research Facilities program will provide new insights into the usefulness of novel high performance computing architectures for science.
- complete reviews on Laboratory Technology Research portfolio (1) to ensure that satisfactory progress has been made toward stated objectives and (2) to assess the scientific quality of the research performed to date.

Significant Accomplishments and Program Shifts

The FY 2001 budget includes substantial enhancements to our research portfolio to build the next generation of high performance computing and communications tools to support the missions of the Office of Science and the Department of Energy in the next century. Increased funding in the areas of advanced scientific computing will be described in more detail in the Mathematical, Information, and Computational Sciences subprogram section.

A new Federally-chartered advisory committee has been established for the Advanced Scientific Computing Research program and has been charged with providing advice on: promising future directions for advanced scientific computing research; strategies to couple advanced scientific computing research in 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.

The ASCR program builds on decades of leadership in high performance computing. Some of the pioneering accomplishments of this program are:

Mathematical, Information, and Computational Sciences (MICS)

- **Established First National Supercomputer Center.** In 1974, DOE established the National Magnetic Fusion Energy Computing Center [the predecessor to the National Energy Research Scientific Computing Center (NERSC)], and pioneered the concept of remote, interactive access to supercomputers. Before this time, scientists using supercomputers had to travel to the location of the computer to make use of it. In addition, users were only able to use these computers by submitting jobs and waiting for hours or days to see the output. The Mathematical, Information, and Computational Sciences (MICS) subprogram developed the first interactive operating system for supercomputers, Cray Time Sharing System (CTSS), as well as a nationwide network to allow remote users to have effective access to the computers. This operating system revolutionized access to supercomputers by enabling users to monitor their jobs as they executed. When the National Science Foundation (NSF) initiated its Supercomputer Centers program in the 1970's, the CTSS operating system was adopted by the San Diego Supercomputing Center and the National Center for Supercomputing Applications to enable users to access NSF's first CRAY machines.
- **Laid Mathematical Foundations for High Performance Computing: Numerical Linear Algebra Libraries.** Today's high performance scientific computations rely on high performance, efficient libraries of numerical linear algebra software. These libraries, which are the core of

numerical efforts in the solution of differential and integral equations LINPACK, EISPAC, LAPACK, SCALAPACK are the direct result of decades of DOE funding of basic research in this area. These libraries are used by thousands of researchers worldwide and are a critical part of the world's scientific computing infrastructure.

- **Developed High Speed Interconnects for Supercomputers: High Performance Parallel Interface (HiPPI).** In order to develop a standard interface between supercomputers and other devices, such as disk arrays and archival tape systems, and visualization computers, DOE laboratories developed the high performance network interface (HiPPI) and led a consortium of vendors to make it the industry standard for the highest bandwidth interconnects between computers and peripheral devices. This advance required the solution of many problems in high speed signaling, data parallelism and high speed protocol design had to be understood to enable this advance.
- **Led the Transition to Massively Parallel Supercomputing: Parallel Virtual Machine (PVM) and Message Passing Interface (MPI).** DOE researchers developed PVM and MPI to enable scientists to make effective use of networks of workstations and massively parallel computers. Both of these software packages have become standards in the industry and are implemented by virtually all of the high performance computer manufacturers in the world. Both of these developments were enabled by over a decade of basic research in message passing and distributed computing supported by DOE along with many experiments to apply these techniques to real scientific problems.
- **Contributed to the Development of the Internet: Slow Start Algorithm for the Transmission Control Protocol (TCP).** Transmission Control Protocol (TCP) part of TCP/IP (Internet Protocol) is responsible for ensuring that packets arrive at their destination. In 1987, as DOE and the other Federal agencies were interconnecting their networks to form the core of the Internet, critical parts of the infrastructure began to fail. There was concern that this represented a fundamental flaw in the TCP/IP architecture; however, a researcher at LBNL applied ideas from fluid flow research to understand the problem and develop a solution. This new TCP algorithm was incorporated in virtually every commercial version of Internet software within six months and enabled the Internet to scale from a small research network to today's worldwide infrastructure.

Building on this long history of accomplishments, principal investigators of the Advanced Scientific Computing Research program this year received recognition through numerous prizes, awards, and honors. A sample of the significant accomplishments and awards produced by the program this year is given below.

Mathematical, Information, & Computational Sciences

- **Parallel Computational Oil Reservoir Simulator.** To meet the Nation's energy needs, the United States oil and gas industry must continue to advance the technology used to extract oil and gas from both new and old fields. Until recently, most drilling and recovery activities were based on past practices that often lacked a sound scientific basis. Computer scientists at Argonne National Laboratory, in collaboration with petroleum engineers at the University of Texas at Austin, have recently developed a software package capable of simulating the flow of oil and gas in reservoirs. These codes, which are based on software tools designed at Argonne, are able to run on a variety of computer platforms, including massively parallel systems with hundreds and even thousands of processors. The software codes will enable the oil and gas industry to lower exploration and drilling costs and enhance the yield of oil from new and old fields alike.
- **Predictability Research Program.** Understanding the behavior of solids, liquids and gases under extreme conditions of temperature and pressure is often the key to understanding complex physical

systems that are critical to a number of the missions of the Department of Energy. The physical conditions under which the devices operate are often so extreme that it is not possible to perform laboratory experiments to validate the design of the devices. Faced with such limitations scientists and engineers are turning more and more to the use of high-speed computers to simulate the behavior of matter under conditions that are not amenable to experimental verification. Under funding from the new MICS Predictability research program a multidisciplinary team of researchers from the Los Alamos and Sandia National Laboratories has performed highly accurate simulations of shockwave-induced fluid instabilities (that are known as Richtmyer-Meshkov instabilities). The simulations match results from “gas-curtain” experiments also conducted by the team over several physically important parameter ranges that can be measured in the laboratory. Researchers are now computationally exploring the behavior of real systems in crucial parameter ranges that are outside of experimental verifiability. This work has broad applicability to our ability to simulate advanced fluid and combustion systems.

- **Theory of Nonequilibrium Solids.** The melting of solids into liquids is a very common, but poorly understood phenomenon that appears in a host of scientific and engineering problems of importance to the Department of Energy. With the appearance of high speed computers in recent years, scientists have been able to couple simulation to theoretical and experimental investigations of melting phenomena, resulting in advances in our understanding of the underlying physics and material properties of solids undergoing melting. An applied mathematician and a materials scientist at the Oak Ridge National Laboratory discovered three distinct “hidden structures” in the melting of two-dimensional materials. This totally unexpected finding has awakened interest among theorists, and it has set off an intense search for additional structures in both two- and three-dimensional problems. This fundamental discovery was enabled by coupling the expertise of the applied mathematician in numerical methods, the expertise of the materials scientist in developing the equations to describe the system, and access to significant high performance computing resources.
- **High Performance Algorithms for Scientific Simulation.** Many problems in science and engineering involve the complex interplay of forces and effects on different time and length scales. Two significant examples of such nonlinear multi-time, multi-scale phenomena are the interaction of the atmosphere and the oceans in the creation of the global climate and the burning of fossil fuels in engines and other devices. The size and complexity of such problems require the development of fast and efficient algorithms and software that can take advantage of the resolution power of today’s massively parallel computing platforms. Applied mathematicians at the Lawrence Berkeley National Laboratory, working in collaboration with applied mathematicians at the Lawrence Livermore National Laboratory and New York University, have developed adaptive mesh refinement algorithms capable of automatically redistributing grid points in computational regions where significant physics is occurring over small time scales. At finer and finer length scales the continuous flow solver is replaced by a particle method such as Monte Carlo, thus allowing the researchers to accurately resolve phenomena over a broad range of length and time scales. Applications of this work to the Accelerated Strategic Computing Initiative (ASCI) and Office of Science problems are many, although the primary focus of the research is the accurate simulation of diesel combustion in realistic, three-dimensional geometries. The laboratory and academic researchers are working on this project closely with engineers from Caterpillar and Cummins.
- **Real-time Reconstruction of Microtomographic Data at the Advanced Photon Source.** The use of X-rays as a non-destructive tool for investigating the internal structure of materials at the micron length scale has grown rapidly over the last decade due to the advent of synchrotron radiation sources such as the Advanced Photon Source (APS). Unfortunately, while advanced detector technology now allows gigabytes of data to be collected in tens of minutes, the computing technologies required to translate this data into images and hence insight have not kept pace. Recent

work at Argonne National Laboratory and the University of Southern California's Information Sciences Institute (ISI) has produced new techniques that overcome this problem. By using a combination of high-performance networking and computing resources, parallel reconstruction algorithms, and advanced resource management, communication, and collaboration software, the Argonne/ISI team was able to demonstrate quasi-real-time 3-D imaging of samples of an APS tomographic beamline. The results as demonstrated in a live run in early May 1999, are stunning: ten minutes after data collection starts, an initial 3-D image appears on the screens of project scientists both at Argonne and at other institutions. Over the next 20 minutes, this image is progressively refined as more data is obtained. For the first time, scientists can change experimental parameters in the middle of an experiment. The implications for better use of scarce facilities and for higher-quality science are clear. This new capability was made possible by support from the ASCR Grand Challenge program and by the parallel computers of Argonne's Center for Computational Science and Technology; it also makes extensive use of distributed computing and collaboration technologies developed under the DOE2000 computing program.

- **Pacific Northwest National Laboratory Researchers Win Best Paper Award at Supercomputing '98.** A paper authored by scientists from DOE's Pacific Northwest National Laboratory entitled, "An Out-of-Core Implementation of the COLUMBUS Massively-Parallel Multireference Configuration Interaction Program" received the Best Application Paper and the Best Overall Paper awards at the Supercomputing '98 conference on November 12, 1998, in Orlando, FL. The paper describes a novel parallelization approach developed to enable COLUMBUS, a legacy chemistry application, to be run efficiently on massively parallel computer platforms rather than the vector supercomputers for which it was originally written. This work was accomplished using Global Arrays, one of the DOE2000 Advanced Computational Testing and Simulation (ACTS) tools supported by MICS. Global Arrays provide a portable shared-memory programming environment optimized for the nonuniform memory hierarchy of modern computer architectures. The chemistry part of this project was supported by the MICS subprogram under the Phase II Grand Challenge program.
- **Argonne Researchers Win "Best of Show" Award at Supercomputing '98.** A team of Argonne scientists and their collaborators received the High-Performance Computing Challenge "best of show" award at the Supercomputing '98 conference for their work on innovative wide-area applications using the GUSTO high-performance distributed grid testbed. GUSTO (Globus Ubiquitous Supercomputing Testbed Organization) is a prototype for future computational grids that will link supercomputers, scientific instruments, virtual reality environments, and data archives transparently. It uses software developed by the Globus project, a multi-institutional collaborative project centered at Argonne and the University of Southern California's Information Science Institute funded by ASCR.
- **Supercomputing (SC'99) Awards.** Special awards were given to scientists from Argonne National Laboratory and University of Chicago for their achievements in simulating incompressible flows and another special award was given to a team of scientists from NASA and DOE laboratories for their achievements in fluid dynamics simulations.
- **TelePresence Microscopy Video Wins the Prestigious Crystal Award of Excellence.** The TelePresence Microscopy project that is part of the DOE2000 program at Argonne National Laboratory's (ANL) Material Sciences Division and is jointly funded by the Department's Mathematical, Information, and Computational Sciences subprogram and the Basic Energy Sciences program, both part of the Office of Science, has won the Prestigious Communicator's "Crystal Award of Excellence." The video was produced in collaboration with ANL's Materials Science Division, the National Institute of Standards and Technology, and Texas Instruments. The video was also funded under the auspices of the "IDEA" program at Texas Instruments and the Office of

MicroElectronics programs at the National Institute of Standards and Technology. The Communicator's Award is a national competition founded by communications professionals to recognize individuals and companies in the communications field whose talent and creativity achieves a high standard of excellence and serves as a standard for the industry.

- **The Maxwell Prize.** A new international prize in applied mathematics, the Maxwell Prize, has been awarded for MICS supported research at the Applied Mathematics Research program at Lawrence Berkeley National Laboratory. The research involved analysis of problems dominated by complexity, such as turbulence, failure and cracks in solids, flow in porous and inhomogeneous media, and combustion. The work on crack formation provided some of the basic tools used today in failure analysis, especially failure due to fatigue.

Laboratory Technology Research (LTR)

The LTR subprogram received five R&D-100 Awards in 1999 for the following research:

- Argonne National Laboratory, in collaboration with the Association of American Railroads and the Electro-Motive Division of General Motors, has developed a technology that should allow diesel engines to operate more cleanly and efficiently. The technology simultaneously minimizes emission of fine-particle pollution and oxides of nitrogen during combustion. It has been demonstrated in a locomotive diesel, but should apply to all types of diesel engines, including those in trucks, buses, heavy equipment, and cars. Practical and less expensive than alternative technologies, it could end a long-standing struggle with diesel pollution.
- Brookhaven National Laboratory, in collaboration with W.R. Grace, has developed the first product capable of destroying asbestos in installed fireproofing on building columns and beams without reducing the fire-resistive performance of the fireproofing material. The new technique, which is now commercially available, uses a foamy solution sprayed directly onto asbestos-containing fireproofing. The foam chemically digests nearly all of the asbestos fibers, dissolving them into harmless minerals. After being treated, the fireproofing is no longer a regulated material. The new process produces essentially no waste and is expected to save building owners the expense of disposing of regulated waste materials.
- 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 electric energy.
- Pacific Northwest National Laboratory (PNNL), in collaboration with DuPont, has developed a suite of programs for massively parallel computing platforms called the "Molecular Sciences Software Suite (MS3)." The new code has been successful in a number of applications to complex problems in the chemical and biochemical sciences. DuPont has used the technology to study the photochemistry of polymeric and agrochemical systems and for rational design of new dyes.
- PNNL, in collaboration with Finnegan MAT, has developed a novel source for enhanced ion detection. The "electrodynamic ion funnel" focuses ions in gases, greatly improving the sensitivity of analytical devices, such as mass spectrometers, that depend on ion formation and transfer in gases. The concept provides a major breakthrough in the field of electrospray mass spectrometry, which will impact fundamental studies in the biological, chemical, and environmental sciences.

In addition to the R&D-100 Awards, six scientists supported by the LTR subprogram were recipients of the following distinguished awards in 1999:

- A Genius Grant from the MacArthur Foundation for development of a method for tricking cells into expressing non-natural sugars on their surface.

- The 39th Annual G.H.A. Clowes Memorial Award for development of therapeutic approaches to breast cancer.
- The American Physical Society's James C. McGroody Prize for innovations in the growth of diamond and germanium crystals.
- The Humboldt Research Award for work on "lab-on-a-chip" micro devices, capable of carrying out chemical measurements normally performed in a conventional laboratory.
- A Federal Laboratory Consortium Award for work on microbiologically influenced corrosion in industrial environments.
- A Presidential Early Career Award for Scientists and Engineers for development of materials and methods that substantially improve the effectiveness of non-thermal plasma technology in treating nitrogen oxide emissions from vehicles.

In FY 1999, the Laboratory Technology Research subprogram initiated a portfolio of Rapid Access Projects that address research problems of small businesses by utilizing the unique facilities of the Office of Science laboratories. These projects were selected on the basis of scientific, technical and potential commercial merit, using competitive external peer review.

Advanced Energy Projects (AEP)

The Advanced Energy Projects subprogram was terminated in FY 2000.

Scientific Facilities Utilization

The ASCR program request includes $32,278,000 in FY 2001 to support the National Energy Research Scientific Computing (NERSC) Center. This investment will provide computer time for about 2,000 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 the Nation's largest, premier unclassified computing center, 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.

Taking The Next Steps in Scientific Computing, Networking, and Collaboration

The accomplishments of the MICS subprogram in scientific computing and enabling distributed scientific teams to work together were described in the ASCR program mission section above. However, additional investments will be required to enable DOE to take the next steps in scientific simulation and to address the challenges that it faces in simulating the complex multidisciplinary phenomena that lie at the heart of its missions. These investments focus on software issues that must be addressed to support today's high performance computers and future computers with significantly higher performance and complexity. They include funding for existing multi-teraflop computers; geographically-dispersed teams of disciplinary scientists, computer scientists, and applied mathematicians; and the supporting infrastructure. Therefore, in FY 2001 the MICS subprogram will enhance its efforts to produce the scientific computing, networking and collaboration tools that DOE researchers will require to address the scientific challenges of the next decade. These enhancements build on the historic strength of the Department of Energy 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. They also take full advantage of the dramatic increases in computing capabilities being fostered by the *Accelerated Strategic Computing Initiative* (*ASCI*) in the Office of Defense Programs.

Scientific Computing

During the past quarter century computational simulation has dramatically advanced our understanding of the fundamental processes of nature and has been used to gain insights into the behavior of such complex natural and engineered systems as the earth's climate and automobile design. The new generation of terascale computing tools, and the 1,000 times more powerful petascale computing capabilities that are now on the horizon, will enable scientists to dramatically improve their understanding of the fundamental processes in many areas. In addition, these new tools will enable scientists to predict the behavior of many complex natural and engineered systems from a knowledge of the underlying physical, chemical, and biological processes involved. This new capability, to predict the behavior of complex systems based on the properties of their components, will change the way DOE and other government agencies solve their most demanding, mission-critical problems. A workshop held at the National Academy of Sciences in July 1998 identified opportunities for new scientific discovery through advanced computing in all of the programs of the Office of Science. The proposed investments to provide programs in computational biology, materials science, chemistry, climate modeling, fusion energy, and high energy and nuclear physics to realize some of these opportunities are discussed in the budgets of those programs.

However, success in those programs depends on investments in applied mathematics and computer science to provide the algorithms, mathematical libraries, and underlying computer science tools to enable the scientific disciplines to make effective use of terascale computers. Despite considerable progress during the past ten years in making massively parallel computer systems usable for applications, much remains to be done. The next generation computer systems to enable leading-edge applications will have between 5,000 and 10,000 individual computer processors rather than the 500-1,000 processors in today's typical high performance systems. In addition, the internal structure of the computers will become more complex as computer designers are forced to introduce more layers of memory hierarchy to maintain performance and develop new hardware features to support rapid communication and synchronization. The end result five years from now will be hardware systems that, while having their roots in today's systems, will be substantially different and substantially more complex and therefore more challenging to exploit for high performance. These challenges will require substantial improvements in parallel computing tools, parallel I/O (input/output) systems, data management, algorithms, and program libraries that must work together as an integrated software system. In addition to the fundamental research challenges that are implied by this evolution in computer hardware, DOE must integrate the output from successful MICS-supported research projects into integrated sets of software tools that scientists in disciplines such as global climate, materials sciences, or computational biology can build on to address scientific challenges.

The MICS subprogram will address these challenges by establishing a small number of competitively selected partnerships (based on a solictation notice to labs and universities) focused on discovering, developing, and deploying to scientists key enabling technologies. These partnerships, which will be called enabling technology 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 will build on the successful experience of the MICS subprogram in managing the DOE2000 initiative, as well as on the lessons learned in important programs supported by 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 enabling technology centers will have close ties to key scientific applications projects to ensure their success.

Networking and Collaboration

Advances in network capabilities and network-based technologies now make it possible for large geographically-distributed teams to effectively collaborate. This is especially important for the teams using the major experimental facilities, computational resources, and data resources supported by DOE. With leadership from DOE, these geographically distributed laboratories or collaboratories have begun to play an important role in the Nation's scientific enterprise. The importance of collaboratories is expected to increase in the future. However, significant research questions must be addressed if collaboratories are to achieve their potential: to enable remote access to petabyte/year High Energy and Nuclear Physics (HENP) facilities such as the Relativistic Heavy Ion Collider (RHIC) to be the same as "being there;" to provide remote visualization of terabyte to petabyte data sets from computational simulation; and to enable effective remote access to tomorrow's advanced scientific computers.

- First, new capabilities are required in the nationwide scientific networks to support collaboratories. For example, using the current Internet, it would take about 2,500 hours to transmit one day's data from RHIC to one remote site for analysis. Typical RHIC experimental collaborations involve thousands of scientists and hundreds of institutions spread across the country and the world who need access to millions of gigabytes (petabytes) of data (a billion times as much data as a large web page). This situation is very different than data management in the commercial sector where millions of users are moving to web pages. Significant research is needed to enable today's commercial networks to be used for scientific data retrieval and analysis. This includes research on advanced protocols, special operating system services to support very high speed transfers, and advanced network control.
- Second, research is needed to understand how to integrate the large number of network devices, network-attached devices, and services that collaboratories require. Examples of the components and services that need to be integrated include: network resources, data archives on tape, high performance disk caches, visualization and data analysis servers, authentication and security services, and the computer on a scientist's desk. All of these physical and software services must be tied together by common software framework building blocks or "middleware" to enable the collaboratories of the future to succeed.

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.

Enhancements to Computing and Networking Facilities

To realize the scientific opportunities, enhancements to the Office of Science's computing and networking facilities are also required. The current computers at NERSC provide less than half of the computer resources that were requested last year. This pressure on the facility 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 is 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.

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 for basic research in: Software, Scalable Information Infrastructure, High End Computing, and Socio-Economic and Workforce Impacts, as well as 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 enhanced 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. In addition, through NERSC and the Advanced Computing Research Facilities, the enhanced MICS subprogram will provide the most powerful high-end computers available to the Nation's scientific and engineering communities.

Funding of Contractor Security Clearances

In FY 1999, the Department divided the responsibility for obtaining and maintaining security clearances. The Office of Security Affairs, which was responsible for funding all Federal and contractor employee clearances, now pays only for clearances of Federal employees, both at headquarters and the field. Program organizations are now responsible for contractor clearances, using program funds. This change in policy enables program managers to make the decisions as to how many and what level clearances are necessary for effective program execution. In this way, it is hoped that any backlog of essential clearances which are impeding program success can be cleared up by those managers most directly involved. The Office of Science is budgeting $47,000 for estimated contractor security clearances in FY 2000 and FY 2001 within this decision unit.

Workforce Development

The R&D Workforce Development mission is to ensure the supply of computational science and PhD level scientists for the Department and the Nation through graduate student and post doctoral research support. In FY 1999, this program will support 855 graduate students and post doctoral investigators, of which 500 will be supported at Science user facilities.

ASCR will continue the Computational Science Graduate Fellowship Program with the successful appointment of 10 new students to support the next generation of leaders in computational science.

Funding Profile

(dollars in thousands)

	FY 1999 Current Appropriation	FY 2000 Original Appropriation	FY 2000 Adjustments	FY 2000 Current Appropriation	FY 2001 Request
Advanced Scientific Computing Research					
Mathematical, Information, and Computational Sciences	135,364	123,000	-3,929	119,071	169,682
Laboratory Technology Research	15,721	9,000	-188	8,812	12,288
Advanced Energy Projects	2,427	0	0	0	0
Subtotal, Advanced Scientific Computing Research	153,512	132,000	-4,117	127,883	181,970
Use of Prior Year Balances	-1,573[a]	0	0	0	0
General Reduction	0	-2,694	2,694	0	0
Contractor Travel	0	-988	988	0	0
Omnibus Rescission	0	-435	435	0	0
Total, Advanced Scientific Computing Research	151,939[b]	127,883	0	127,883	181,970

Public Law Authorization:

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

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

[a] Share of Science general reduction for use of prior year balances assigned to this program. The total general reduction is applied at the appropriation level.

[b] Excludes $3,735,000 which has been transferred to the SBIR program and $224,000 which has been transferred to the STTR program.

Funding by Site

	FY 1999	FY 2000	FY 2001	$ Change	% Change
	(dollars in thousands)				
Albuquerque Operations Office					
Los Alamos National Laboratory	15,206	11,873	10,560	-1,313	-11.1%
National Renewable Energy Laboratory	127	0	0	0	0.0%
Sandia National Laboratories	5,651	4,798	4,705	-93	-1.9%
Total, Albuquerque Operations Office	20,984	16,671	15,265	- 1,406	-8.4%
Chicago Operations Office					
Ames Laboratory	2,239	1,672	1,571	-101	-6.0%
Argonne National Laboratory	19,032	12,187	11,958	-229	-1.9%
Brookhaven National Laboratory	2,023	1,811	1,504	-307	-17.0%
Fermi National Accelerator Laboratory	213	60	200	+140	+233.3%
Princeton Plasma Physics Laboratory	121	45	200	+155	+344.4%
Chicago Operations Office	19,746	11,001	10,265	-736	-6.7%
Total, Chicago Operations Office	43,374	26,776	25,698	-1,078	-4.0%
Oakland Operations Office					
Lawrence Berkeley National Laboratory	57,969	53,865	64,457	+10,592	+19.7%
Lawrence Livermore National Laboratory	3,620	3,210	3,160	-50	-1.6%
Stanford Linear Accelerator Center	1,052	375	450	+75	+20.0%
Oakland Operations Office	5,176	2,474	2,179	-295	-11.9%
Total, Oakland Operations Office	67,817	59,924	70,246	+10,322	+17.2%
Oak Ridge Operations Office					
Oak Ridge Inst. For Science and Education	169	20	20	0	0.0%
Oak Ridge National Laboratory	13,392	7,584	6,719	-865	-11.4%
Thomas Jefferson National Accelerator Facility	151	50	200	+150	+300.0%
Oak Ridge Operations Office	17	42	0	-42	-100.0%
Total, Oak Ridge Operations Office	13,729	7,696	6,939	-757	-9.8%
Richland Operations Office					
Pacific Northwest National Laboratory	4,312	2,602	2,210	-392	-15.1%
Washington Headquarters	3,296	14,214	61,612	+47,398	+333.5%
Subtotal, Advanced Scientific Computing Research	153,512	127,883	181,970	+54,087	+42.3%
Adjustment	-1,573[a]	0	0	0	0.0%
Total, Advanced Scientific Computing Research	151,939[b]	127,883	181,970	+54,087	+42.3%

[a] Share of Science general reduction for use of prior year balances assigned to this program. The total general reduction is applied at the appropriation level.

[b] Excludes $3,735,000 which has been transferred to the SBIR program and $224,000 which has been transferred to the STTR program.

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 the materials scientific application pilot project, which focuses on applying advanced computing to problems in microstructural defects, alloys, and magnetic materials, and in computer science. 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 facility. The Advanced Computing Research Facility (ACRF) at ANL focuses on advanced computers in the IBM-SP family of technologies as well as the interaction of those architectures with advanced visualization hardware. 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 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 as well as supporting an advanced computing research facility. The Advanced Computing Research Facility (ACRF) at LBNL currently focuses on very large scale computing on hardware in the T3E architecture from SGI-Cray including issues of distributing jobs over all the processors efficiently and the associated system management issues. 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 a 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.

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 as well as supporting an advanced computing research facility. The Advanced Computing Research Facility (ACRF) at LANL focuses on a progression of technologies from SGI - Cray involving Origin 2000 Symmetric Multiprocessor Computers linked with HiPPI crossbar switches. This series of research computers has been given the name “Nirvana Blue.”

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. 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 wire, 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. 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 simulation of glass production, interactions of biological polymers with model surfaces, and characterization of micro-organisms 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 Tonapah, 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.

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 enabling technology 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 and developing the advanced computing and communications tools and operating the high performance computing and network facilities that researchers need to analyze, model, simulate, and — most importantly — predict complex phenomena of importance to the Office of Science and to the Department of Energy. The MICS subprogram supports fundamental research and research facilities in all of the areas in which MICS supports research:

- **Applied Mathematics.** This includes research on the underlying mathematical understanding and numerical algorithms to enable effective description and prediction of physical systems such as fluids, magnetized plasmas, or protein molecules. This includes, for example, methods for solving large systems of partial differential equations on parallel computers, techniques for choosing optimal values for parameters in large systems with hundreds to hundreds of thousands of parameters, improving our understanding of fluid turbulence, and developing techniques for reliably estimating the errors in simulations of complex physical phenomena.
- **Computer Science.** This includes research in computer science to enable large scientific applications through advances in massively parallel computing such as very lightweight operating systems for parallel computers, distributed computing such as development of the Parallel Virtual Machine (PVM) software package which has become an industry standard, and large scale data management and visualization. The development of new computer and computational science techniques will allow scientists to use the most advanced computers without being overwhelmed by the complexity of rewriting their codes every 18 months.
- **Networking.** This includes research in high performance networks and information surety required to support high performance applications – protocols for high performance networks, methods for measuring the performance of high performance networks, and software to enable high speed connections between high performance computers and networks. The development of high speed communications and collaboration technologies will allow scientists to view, compare, and integrate data from multiple sources remotely.

MICS also operates supercomputer and network facilities that are available to researchers 24 hours a day, 365 days a year. The requirements far exceed the current state-of-the-art; furthermore, the requirements far exceed the tools that the commercial marketplace will deliver. For this reason, 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 test 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.

Performance Measures

- Facilities, including the National Energy Research Scientific Computing Center (NERSC) and ESnet, will be operated within budget and successfully meet user needs and satisfy overall SC program requirements where, specifically, NERSC will deliver 3.6 Teraflop capability by the end of FY 2001 to support DOE's science mission.
- Conduct regular peer review and merit evaluation based on the principles set down in 10 CFR Part 605 for grants and cooperative agreements, with all research projects reviewed at least once and no project extending more than four years without review.
- Support the Computational Science Graduate Fellowship Program with the successful appointment of 10 new students to support the next generation of leaders in computational science for DOE and the Nation.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Mathematical, Computational, and Computer Sciences Research	48,896	46,086	73,030	+26,944	+58.5%
Advanced Computation, Communications Research and Associated Activities	86,468	69,996	92,441	+22,445	+32.1%
SBIR/STTR	0[a]	2,989	4,211	+1,222	+40.9%
Total, Mathematical, Information, and Computational Sciences	135,364	119,071	169,682	+50,611	+42.5%

[a] Excludes $3,274,000 which has been transferred to the SBIR program and $196,000 which has been transferred to the STTR program.

Detailed Program Justification

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001

Mathematical, Computational, and Computer Sciences Research

- **Applied Mathematics:** Research 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 because of the potential of improved mathematical techniques to enable large computational simulations. In fact, the contribution of improved mathematical methods to advancing computer simulation exceeds the contribution due to speedup in the underlying hardware. This activity supports research at DOE laboratories, universities, and private companies. Many of the projects supported by this activity are partnerships between researchers at universities and DOE laboratories. To accomplish its goals, the program supports research in a number of areas including: Mathematical Physics including string theory, superstring theory, geometry of space-time, and quantum effects; Ordinary and Partial Differential Equations including numerical methods, high performance algorithms, massively parallel algorithms, novel gridding schemes, numerical linear algebra, iterative methods, sparse solvers, and dense solvers; 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; Fluid Dynamics including compressible, incompressible and reacting flows, turbulence modeling, and multiphase flows; Dynamical Systems including chaos-theory and control, and bifurcation theory; Programming and Optimization including linear and nonlinear programming, interior-point methods, and discrete and integer programming; and Geometric and Symbolic Computing including minimal surfaces and automated theorem proving. The FY 2001 budget includes the continuation of work initiated in FY 1999 to develop the mathematical basis for modeling and simulating complex stochastic phenomena of the type that arise in vital DOE areas such as global climate modeling,

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
and environmental remediation. This research also provides the basis for Defense Programs' investments in understanding the predictability of stockpile stewardship simulation. The FY 2001 budget also includes an increased level of funding for the Computational Sciences Graduate Fellowship program ($2,000,000) and funds for the competitive selection (based on a solicitation notice to labs and universities) of two enabling technology centers focused on algorithms and mathematical libraries for critical DOE applications on terascale computers ($7,700,000)...	22,564	23,354	33,054
■ **Computer Science:** Research in computer science to enable large scientific applications. This activity is critical to DOE because its 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. 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. This research is carried out by researchers at DOE laboratories and universities, often working together in partnerships. The enhancements to this activity in FY 2001 will permit the establishment of a small number of competitively selected enabling technology centers to address critical computer science and systems software issues for terascale computers including: scalable open source operating systems; tools for analyzing and debugging scientific simulation software that uses thousands of processors; and the development of data management and visualization software capable of handling terabyte scale data sets extracted from petabyte scale data archives. ($7,476,000) These enabling technology centers are a critical component in DOE's strategy for taking the next steps in scientific simulation and modeling...	14,000	14,000	21,476

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
■ **Advanced Computing Software Tools:** 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, which 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. The initial goal of this program element was to develop foundational tools (math libraries, runtime systems, etc.) that will have a useful life spanning many generations of computer hardware. From the experience gained with end user application scientists applying these tools, it has become clear that to promote wide usage across the scientific community the tools must also be robust and easy to use. Since many of the tools needed in the high performance arena have no commercial market, enabling technology centers will provide a means for focused investment to deploy these tools to the scientific community. These competitively selected centers will focus research in several areas that include software frameworks, problem solving environments, distributed computing and collaboration technologies, as well as visualization and data management. A substantial increase in this effort is provided to support this goal.	5,000	5,000	9,000
■ **Scientific Applications Pilot Projects:** This research applies computational techniques and tools developed in the Advanced Computing Software Tools effort to basic research problems in order to test the usefulness of current advanced computing research, transfer the results of this research to the scientific disciplines, and help define promising areas for future research. In FY 2000, Grand Challenge projects initiated in FY 1991 as part of DOE's component of the Federal High Performance Computing and Communications program were phased out. The FY 2001 funding for this activity will allow the initiation of a small number of new			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
pilot projects. The selection of these projects will be based on open, competitive processes. These pilot projects will be tightly coupled to the enabling technology centers (described above in computer science) and 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.	7,332	3,732	9,500
Total Mathematical, Computational, and Computer Sciences Research..	48,896	46,086	73,030
Advanced Computation, Communications Research, and Associated Activities			
■ **Networking:** Research in high performance computer networks and information security required to support high performance computer applications — protocols for high performance networks, methods for measuring the performance of high performance networks, and software to enable high speed connections between high performance computers and both local area and wide area networks. In addition, this activity supports research in network protocols that enable applications to request, and be guaranteed, minimum acceptable levels of network capability. The enhanced level of effort in this activity in FY 2001 will enable research in the high performance "middleware," software that applications need to couple effectively to advanced network services...	4,500	6,000	7,500
■ **Collaboratory Tools:** This research uses the results of fundamental research on computer science and networking to develop an integrated set of software tools to enable scientists to remotely access and control facilities and share data in real time. These tools are necessary to provide a new way of organizing and performing scientific work that offers the potential for increased productivity and efficiency. This research includes, for example, 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. Having demonstrated feasibility of the security architecture on a small scale, an additional investment is needed to support the integration of			

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
collaboratory tools with advanced networking services in a research setting. In this way, security features can be integrated into more end user applications or collaboratory tools. In addition, all these can be demonstrated on a large user base. Other examples of research in collaboratory tools include the development of a modular electronic notebook prototype for the sharing of scientific results, data from scientific instruments and design of scientific procedures; and the development of tools to manage distributed collaborations where videoconferencing, whiteboards and other shared applications are important. Shared controls for remote, collaborative control of visualizations are also being investigated.	3,000	3,000	5,600

- **National Collaboratory Pilot Projects:** R&D to test, validate, and apply collaboratory tools in partnership with other DOE programs. It is important to demonstrate and test the benefits of collaboratory tools technology in order to promote its widespread use. The two continuing pilot projects are: (1) the Materials MicroCharacterization Collaboratory, a partnership with the Basic Energy Sciences program and Energy Efficiency and Renewable Energy to provide remote access to facilities located at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, Argonne National Laboratory, and the National Institute of Standards and Technology, and the University of Illinois for electron beam microcharacterization of materials; and (2) the Diesel Combustion Collaboratory, a partnership with Basic Energy Sciences, Energy Efficiency and Renewable Energy, and three U.S. manufacturers of diesel engines, to link researchers at Sandia National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and the University of Wisconsin with researchers at industrial laboratories in Indiana and Michigan to develop the next generation of clean diesel engines. As communications technologies and middleware developments converge and lead to new services, a closer coupling needs to be made to the end scientific applications. Hence an increase is made for R&D to test, validate, and apply wide area data intensive collaborative computing technologies in partnerships between end user application scientists, developers of collaboration tools and other middleware, and network researchers. These

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
partnerships will be focused to develop user environments where collaboration is ubiquitous and distributed computing is seamless and transparent for DOE mission applications such as High Energy and Nuclear Physics Data, remote visualization of simulation results, and advanced collaboratories.	3,000	5,000	11,000
■ **National Energy Research Scientific Computing Center (NERSC):** NERSC, located at LBNL, provides high performance computing for investigators supported by the Office of Science. The Center serves 2,000 users working on about 700 projects; 35 percent of users are university based, 60 percent are in National Laboratories, and 5 percent are in industry. 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 large IBM SP computer whose initial installation was completed in early FY 2000 in a fully competitive procurement. The additional funding in FY 2001 will enable this computer to be enhanced to over 5 teraflops peak performance. This represents nearly a 40% increase over the capability that would have been attainable without the increase in funding. These computational resources will be integrated by a common high performance file storage system that facilitates interdisciplinary collaborations Related requirements for capital equipment and general plant projects (GPP) funding are also supported..	26,500	26,500	32,278
■ **Advanced Computing Research Facilities (ACRFs):** ACRFs support advanced computational hardware testbeds for scientific application pilot projects and fundamental research in applied mathematics and computer science. ACRFs are located at Los Alamos National Laboratory (Nirvana Blue partnership with the DOE Biological and Environmental Research (BER) program and Defense Programs (DP), based on SGI/Cray Technology); Argonne National Laboratory (IBM-SP); and Lawrence Berkeley National Laboratory (SGI/Cray T3E and IBM SP). Smaller evaluation efforts based on experimental clusters of Compaq-Alpha technology and Intel based processors are supported at ORNL and ANL. Because many of the issues to be investigated only appear in the computer systems at			

	(dollars in thousands)	
FY 1999	FY 2000	FY 2001

	FY 1999	FY 2000	FY 2001
significantly larger scale than the computer manufacturers' commercial design point, these facilities must procure the largest scale systems that can be afforded and develop software to manage and make them useful. In addition, the ACRFs, taken together, must have a full range of different 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, all of these systems are managed as research programs and not as information technology investments. Related capital equipment needs such as high speed disk storage systems, archival data storage systems and high performance visualization hardware are also supported. An additional $2,027,000 will allow for experiments with one additional computer architecture for a high-priority DOE application. The site will be determined competitively.	20,079	13,749	15,776

- **Energy Sciences Network (ESnet):** ESnet provides worldwide access to the Office of Science facilities, including: advanced light sources; neutron sources; particle accelerators; fusion reactors; spectrometers; ACRFs; and other leading-edge science instruments and facilities. ESnet provides the communications fabric that links DOE researchers to one another and forms the basis for fundamental research in networking, enabling R&D in collaboratory tools, and applications testbeds such as the national collaboratory pilot projects. To provide these facilities, ESnet management at LBNL contracts with commercial vendors for advanced communications services including Asynchronous Transfer Mode (ATM) and Wave Division Multiplexing (WDM). ESnet management provides system integration to provide a uniform interface to these services for DOE laboratories. In addition, ESnet management is responsible for the interfaces between the network fabric it provides and the worldwide Internet including the University Corporation for Advanced Internet Development (UCAID) Abilene network that provides high performance connections to many research universities. One

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
reason that ESnet, in the words of the 1998 external review committee, is able to provide the capabilities and services to its users "at significantly lower budgets than other agencies" is its management structure with strong user and site coordination committees. This management structure is built on DOE's experience in operating large user facilities. The enhanced funding in FY 2001 will support an advanced network testbed to enable research in collaboratory tools and pilots as well as the increases in bandwidth needed to support terascale computers and the next generation of petabyte/year scale experimental facilities. Related capital equipment needs are also supported such as high speed network routers, ATM switches, and network management and testing equipment.	14,787	15,747	20,287
■ **Next Generation Internet (NGI):** This program focused on goals of the government-wide program and supported efforts to develop, test, and validate networking technologies that DOE mission-critical applications require. Core aspects of this long-standing research are supported within the MICS subprogram as they have been since the beginning of the HPCC program in FY 1991	14,602	0	0
Total, Advanced Computation, Communications Research, and Associated Activities	86,468	69,996	92,441

SBIR/STTR

■ In FY 1999, $3,274,000 and $196,000 were transferred to the SBIR and STTR programs, respectively. The FY 2000 and FY 2001 amounts are the estimated requirement for the continuation of the SBIR and STTR programs.	0	2,989	4,211
Total, Mathematical, Information, and Computational Sciences	135,364	119,071	169,682

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Mathematical, Computational, and Computer Sciences Research	
■ Increase in the Computational Sciences Graduate Fellowship program and funds for the competitive selection of two enabling technology centers focused on algorithms and mathematical libraries for critical DOE applications on terascale computers.	+9,700
■ Increase in computer science for enabling technology centers - a critical component in DOE's strategy for taking the next steps in computational modeling and simulation.	+7,476
■ Increase in advanced computing software tools for enabling technology centers, for a focused investment to deploy tools to the scientific community.	+4,000
■ Increase in scientific applications pilot projects to allow the initiation of several new pilot projects that will be tightly coupled to the enabling technology centers in applied mathematics and computer science.	+5,768
Total Mathematical, Computational, and Computer Sciences Research	+26,944
Advanced Computation, Communications Research, and Associated Activities	
■ Increase in networking to enable research in the high performance "middleware" software that applications need to couple effectively to advanced network services.	+1,500
■ Increase in collaboratory tools to support the integration of collaboratory tools with advanced networking services in a research setting.	+2,600
■ Increase in national collaboratory pilot projects to test, validate, and apply collaboratory tools in partnership with other DOE programs.	+6,000
■ Increase in NERSC funding for computer enhancement.	+5,778
■ Increase in support for Advanced Computing Research Facilities (ACRFs)	+2,027
■ Increase in support of ESnet operations for an advanced network testbed and access to multi-teraflop computers.	+4,540
Total, Advanced Computation, Communications Research, and Associated Activities	+22,445
SBIR/STTR	
■ Increase in SBIR/STTR due to increase in operating expenses.	+1,222
Total Funding Change, Mathematical, Information, and Computational Sciences	+50,611

Laboratory Technology Research

Mission Supporting Goals and Objectives

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

An important component of the Department's strategic goals is 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 program component provides rapid access by small business 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 three critical areas of DOE mission-related research: advanced materials processing and utilization, intelligent processes and controls, and energy-related applications of biotechnology.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Laboratory Technology Research...........	12,753	8,578	11,963	+3,385	+39.5%
SBIR/STTR	0[a]	234	325	+91	+38.9%
Congressional Direction	2,968	0	0	0	0.0%
Total, Laboratory Technology Research..	15,721	8,812	12,288	+3,476	+39.4%

[a] Excludes $399,000 which has been transferred to the SBIR program and $24,000 which has been transferred to the STTR program.

Detailed Program Justification

	(dollars in thousands)		
	FY 1999	FY 2000	FY 2001
Laboratory Technology Research			
■ This activity supports research to advance the fundamental science at the Office of Science 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 approximately 70 projects and emphasizes the following topics: advanced materials processing and utilization, intelligent processes and controls, and energy-related applications of biotechnology. Efforts underway include the exploration of (1) a unique direct casting technology for production of lower-cost, better-performing titanium wire for use in the aerospace and automotive industries; (2) the identification of plants that can be used in freshwater, aquatic, and edge environments to remove contaminants from sediment, without substantial alteration of the ecosystems; and (3) the characterization of polymer composite matrix materials, using electron beam curing, to produce stronger, lighter, and more durable materials with much lower energy demands. 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) web-based energy performance benchmarking to improve the energy efficiency of buildings; (2) a magnetic particle process to separate selectively iron and chromium from plating tank solutions, thereby improving plating efficiency and minimizing waste disposal cost; and (3) tools for the genetic manipulation of *Streptococcus pneumoniae* to demonstrate gene function and to identify novel genetic elements in transcription, which could lead to improved antibiotics for respiratory disease.	12,753	8,578	11,963

	FY 1999	FY 2000	FY 2001
	(dollars in thousands)		
SBIR/STTR			
In FY 1999, $399,000 and $24,000 were transferred to the SBIR and STTR programs, respectively. The FY 2000 and FY 2001 amounts are the estimated requirement for the continuation of the SBIR and STTR programs.........................	0	234	325
Congressional Direction			
Funds the University of Southwestern Louisiana (per FY 1997 Congressional Direction)...	2,968	0	0
Total, Laboratory Technology Research....................................	15,721	8,812	12,288

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Laboratory Technology Research	
■ Increase in multiyear technology research partnership projects....................	+3,385
SBIR/STTR	
■ Increase in SBIR/STTR due to increase in operating expenses.	+91
Total Funding Change, Laboratory Technology Research	+3,476

Advanced Energy Projects

Mission Supporting Goals and Objectives

The Advanced Energy Projects (AEP) subprogram funded research that established the feasibility of novel, energy-related concepts that span the Department's energy mission and goals. Funded projects were based on innovative ideas that spanned multiple scientific and technical disciplines and did not fit into any other DOE program area. A common theme for each project was the initial linkage of new research results to an energy application with a potentially significant payoff. Typically, AEP supported projects up to a level of about $250,000 per year for a period of about 3 years. Projects were selected from proposals submitted by universities and national laboratories. Funding criteria emphasized scientific merit as judged by external peer review.

Funding Schedule

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
Advanced Energy Projects	2,427	0	0	0	0.0%
SBIR/STTR	0[a]	0	0	0	0.0%
Total, Advanced Energy Projects	2,427	0	0	0	0.0%

Detailed Program Justification

(dollars in thousands)

	FY 1999	FY 2000	FY 2001
Advanced Energy Projects			
■ Support for high-risk, high-payoff research at universities and national laboratories established the feasibility of novel energy related concepts that were at an early stage of scientific definition. Final funds for these projects were provided in FY 1999	2,427	0	0
SBIR/STTR			
■ In FY 1999, $62,000 and $4,000 were transferred to the SBIR and STTR programs, respectively.	0	0	0
Total, Advanced Energy Projects	2,427	0	0

[a] Excludes $62,000 which has been transferred to the SBIR program and $4,000 which has been transferred to the STTR program.

Explanation of Funding Changes from FY 2000 to FY 2001

	FY 2001 vs. FY 2000 ($000)
Advanced Energy Projects	
■ The AEP program was terminated in FY 2000.	0
Total Funding Change, Advanced Energy Projects	0

Capital Operating Expenses & Construction Summary

Capital Operating Expenses

(dollars in thousands)

	FY 1999	FY 2000	FY 2001	$ Change	% Change
General Plant Projects.......................	70	0	2,000	+2,000	+100.0%
Capital Equipment (total)...................	8,798	6,275	8,775	+2,500	+39.8%
Total, Capital Operating Expenses......	8,868	6,275	10,775	+4,500	+71.7%

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

(dollars in thousands)

	Total Estimated Cost (TEC)	Prior Year Approp-riations	FY 1999	FY 2000	FY 2001	Accept-ance Date
Archival Systems Upgrade – LBNL.........	2,000	0	0	2,000	0	FY 2002
Distributed Visualization Server – LBNL ..	2,500	0	0	0	2,500	FY 2001
Total, Major Items of Equipment		0	0	2,000	2,500	