DOE/CF-005
Volume 4

# DEPARTMENT OF ENERGY

# FY 2007 CONGRESSIONAL BUDGET REQUEST

## SCIENCE
## NUCLEAR WASTE DISPOSAL
## DEFENSE NUCLEAR WASTE DISPOSAL

## DEPARTMENTAL ADMINISTRATION
## INSPECTOR GENERAL
## WORKING CAPITAL FUND

FEBRUARY 2006

VOLUME 4

OFFICE OF CHIEF FINANCIAL OFFICER

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# Volume 4

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The Department of Energy's FY 2007 Congressional Budget justification is available on the Office of Chief Financial Offier/CFO homepage at http://www.mbe.doe.gov/budget/

# Department of Energy
## Appropriation Account Summary
(dollars in thousands - OMB Scoring)

| | FY 2005 Current Approp. | FY 2006 Current Approp. | FY 2007 Congressional Request | FY 2007 vs. FY 2006 $ | FY 2007 vs. FY 2006 % |
|---|---|---|---|---|---|
| **Discretionary Summary By Appropriation** | | | | | |
| Energy And Water Development, And Related Agencies | | | | | |
| Appropriation Summary: | | | | | |
| Energy Programs | | | | | |
| Energy supply and Conservation | 1,801,815 | 1,812,627 | 1,923,361 | +110,734 | +6.1% |
| Fossil energy programs | | | | | |
| Clean coal technology | -160,000 | -20,000 | —— | +20,000 | +100.0% |
| Fossil energy research and development | 560,852 | 592,014 | 469,686 | -122,328 | -20.7% |
| Naval petroleum and oil shale reserves | 17,750 | 21,285 | 18,810 | -2,475 | -11.6% |
| Elk Hills school lands fund | 36,000 | 84,000 | —— | -84,000 | -100.0% |
| Strategic petroleum reserve | 126,710 | 207,340 | 155,430 | -51,910 | -25.0% |
| Northeast home heating oil reserve | 4,930 | —— | 4,950 | +4,950 | N/A |
| Strategic petroleum account | 43,000 | -43,000 | —— | +43,000 | +100.0% |
| Total, Fossil energy programs | 629,242 | 841,639 | 648,876 | -192,763 | -22.9% |
| Uranium enrichment D&D fund | 495,015 | 556,606 | 579,368 | +22,762 | +4.1% |
| Energy information administration | 83,819 | 85,314 | 89,769 | +4,455 | +5.2% |
| Non-Defense environmental cleanup | 439,601 | 349,687 | 310,358 | -39,329 | -11.2% |
| Science | 3,635,650 | 3,596,391 | 4,101,710 | +505,319 | +14.1% |
| Nuclear waste disposal | 343,232 | 148,500 | 156,420 | +7,920 | +5.3% |
| Departmental administration | 128,598 | 128,519 | 128,825 | +306 | +0.2% |
| Inspector general | 41,176 | 41,580 | 45,507 | +3,927 | +9.4% |
| Total, Energy Programs | 7,598,148 | 7,560,863 | 7,984,194 | +423,331 | +5.6% |
| Atomic Energy Defense Activities | | | | | |
| National nuclear security administration: | | | | | |
| Weapons activities | 6,625,542 | 6,369,597 | 6,407,889 | +38,292 | +0.6% |
| Defense nuclear nonproliferation | 1,507,966 | 1,614,839 | 1,726,213 | +111,374 | +6.9% |
| Naval reactors | 801,437 | 781,605 | 795,133 | +13,528 | +1.7% |
| Office of the administrator | 363,350 | 338,450 | 386,576 | +48,126 | +14.2% |
| Total, National nuclear security administration | 9,298,295 | 9,104,491 | 9,315,811 | +211,320 | +2.3% |
| Environmental and other defense activities: | | | | | |
| Defense environmental cleanup | 6,800,848 | 6,130,447 | 5,390,312 | -740,135 | -12.1% |
| Other defense activities | 687,149 | 635,578 | 717,788 | +82,210 | +12.9% |
| Defense nuclear waste disposal | 229,152 | 346,500 | 388,080 | +41,580 | +12.0% |
| Total, Environmental & other defense activities | 7,717,149 | 7,112,525 | 6,496,180 | -616,345 | -8.7% |
| Total, Atomic Energy Defense Activities | 17,015,444 | 16,217,016 | 15,811,991 | -405,025 | -2.5% |
| Power marketing administrations: | | | | | |
| Southeastern power administration | 5,158 | 5,544 | 5,723 | +179 | +3.2% |
| Southwestern power administration | 29,117 | 29,864 | 31,539 | +1,675 | +5.6% |
| Western area power administration | 171,715 | 231,652 | 212,213 | -19,439 | -8.4% |
| Falcon & Amistad operating & maintenance fund | 2,804 | 2,665 | 2,500 | -165 | -6.2% |
| Colorado River Basins | —— | -23,000 | -23,000 | —— | —— |
| Total, Power marketing administrations | 208,794 | 246,725 | 228,975 | -17,750 | -7.2% |
| Federal energy regulatory commission | —— | —— | —— | —— | —— |
| Subtotal, Energy And Water Development and Related Agencies | 24,822,386 | 24,024,604 | 24,025,160 | +556 | +0.0% |
| Uranium enrichment D&D fund discretionary payments | -459,296 | -446,490 | -452,000 | -5,510 | -1.2% |
| Excess fees and recoveries, FERC | -18,452 | -15,542 | -16,405 | -863 | -5.6% |
| **Total, Discretionary Funding** | **24,344,638** | **23,562,572** | **23,556,755** | **-5,817** | **-0.0%** |

# Science

# Science

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# Science

## Proposed Appropriation Language

For Department of Energy expenses including the purchase, construction and acquisition of plant and capital equipment, and other expenses necessary for science activities in carrying out the purposes of the Department of Energy Organization Act (42 U.S.C. 7101 et seq.), including the acquisition or condemnation of any real property or facility or for plant or facility acquisition, construction, or expansion, and purchase of not to exceed **[**forty-seven**]** *forty-nine* passenger motor vehicles for replacement only, including not to exceed one ambulance and two buses, **[**$3,632,718,000**]** *$4,101,710,000*, to remain available until expended. *(Energy and Water Development Appropriations Act, 2006.)*

## Explanation of Change

Changes are proposed to reflect the FY 2007 funding and vehicle request.

# Science
# Office of Science

## Overview

## Appropriation Summary by Program

(dollars in thousands)

| | FY 2005 Current Appropriation | FY 2006 Original Appropriation | FY 2006 Adjustments | FY 2006 Current Appropriation | FY 2007 Request |
|---|---|---|---|---|---|
| Science | | | | | |
| Basic Energy Sciences | 1,083,616 | 1,146,017 | -11,460[a] | 1,134,557 | 1,420,980 |
| Advanced Scientific Computing Research | 226,180 | 237,055 | -2,371[a] | 234,684 | 318,654 |
| Biological and Environmental Research | 566,597 | 585,688 | -5,857[a] | 579,831 | 510,263 |
| High Energy Physics | 722,906 | 723,933 | -7,239[a] | 716,694 | 775,099 |
| Nuclear Physics | 394,549 | 370,741 | -3,707[a] | 367,034 | 454,060 |
| Fusion Energy Sciences | 266,947 | 290,550 | -2,906[a] | 287,644 | 318,950 |
| Science Laboratories Infrastructure | 37,498 | 42,105 | -421[a] | 41,684 | 50,888 |
| Science Program Direction | 154,031 | 160,725 | -1,607[a] | 159,118 | 170,877 |
| Workforce Development for Teachers and Scientists | 7,599 | 7,192 | -72[a] | 7,120 | 10,952 |
| Safeguards and Security | 72,773 | 74,317 | -687[a] | 73,630 | 76,592 |
| Small Business Innovation Research/ Small Business Technology Transfer | 113,621[b] | — | — | — | — |
| Subtotal, Science | 3,646,317 | 3,638,323 | -36,327 | 3,601,996 | 4,107,315 |
| Less use of prior year balances | -5,062 | — | — | — | — |
| Less security charge for reimbursable work | -5,605 | -5,605 | — | -5,605 | -5,605 |
| Total, Science | 3,635,650 | 3,632,718 | -36,327 | 3,596,391 | 4,101,710 |

### Preface

As part of the President's American Competitiveness Initiative, the Office of Science (SC) request for Fiscal Year (FY) 2007 is $4,101,710,000; an increase of $505,319,000, or 14.1%, from the FY 2006 appropriation. The request funds investments in basic research that are critical to both the future economic competitiveness of the United States and to the success of Department of Energy (DOE) missions in national security and energy security; advancement of the frontiers of knowledge in the physical sciences and areas of biological, environmental, and computational sciences; and provision of world-class research facilities for the Nation's science enterprise.

SC provides the basic research that underpins the Department's technically complex missions. Part of this support is in the form of large-scale scientific user facilities that form the backbone of modern research. The suite of forefront facilities includes the world's highest energy proton accelerator—Fermi National Accelerator Laboratory's (Fermilab's) Tevatron—and the soon to be operational Spallation

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[a] Reflects a rescission in accordance with P.L. 109–148, the Emergency Supplemental Appropriations Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006.

[b] Includes $77,842,000 reprogrammed within SC and $35,779,000 transferred from other DOE programs.

Neutron Source (SNS). SC facilities represent a continuum of unique capabilities that meet the needs of a diverse set of nearly 20,000 researchers each year. For example, the National Synchrotron Light Source (NSLS) began ultraviolet operations in 1982 and, initially, primarily enabled physical science research. However, through the 1990's the numbers of researchers from the life sciences rapidly grew as the characteristics of this facility better suited the needs of researchers who study protein structure. Today, the NSLS is playing a major role in the Protein Structure Initiative, a national effort to find the three-dimensional shapes of a wide range of proteins, while also providing a suite of beamlines to the soon to be available Center for Functional Nanomaterials and a host of other research efforts.

Within the Science appropriation, SC has 10 programs: Basic Energy Sciences (BES), Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER), High Energy Physics (HEP), Nuclear Physics (NP), Fusion Energy Sciences (FES), Science Laboratories Infrastructure (SLI), Science Program Direction (SCPD), Workforce Development for Teachers and Scientists (WDTS), and Safeguards and Security (S&S).

This Overview will describe Strategic Context, Mission, Benefits, Strategic Goals, and Funding by General Goal. These items together put the appropriation request in perspective. The Annual Performance Results and Targets, Means and Strategies, and Validation and Verification sections address how the goals will be achieved and how performance will be measured. Finally, this Overview will address the Research and Development (R&D) Investment Criteria, Program Assessment Rating Tool (PART), and Significant Program Shifts.

**Strategic Context**

Following publication of the Administration's National Energy Policy, the Department developed a Strategic Plan that defines its mission, four strategic goals for accomplishing that mission, and seven general goals to support the strategic goals. Each appropriation has developed quantifiable goals to support the general goals. Thus, the "goal cascade" is the following:

Department Mission ➡ Strategic Goal (25 yrs) ➡ General Goal (10–15 yrs) ➡ Program Goal (Government Performance and Results Act [GPRA] Unit) (10–15 yrs).

To provide a concrete link between budget, performance, and reporting, the Department developed a "GPRA Unit" concept. Within DOE, a GPRA Unit defines a major activity or group of activities that support the core mission and aligns resources with specific goals. Each GPRA Unit has completed or will complete a PART. A unique program goal was developed for each GPRA unit. A numbering scheme has been established for tracking performance and reporting.

The goal cascade accomplishes two things. First, it ties major activities for each program to successive goals and, ultimately, to DOE's mission. This helps ensure the Department focuses its resources on fulfilling its mission. Second, the cascade allows DOE to track progress against quantifiable goals and to tie resources to each goal at any level in the cascade. Thus, the cascade facilitates the integration of budget and performance information in support of the GPRA and the President's Management Agenda (PMA).

Another important component of our strategic planning—and the PMA—is use of the Administration's R&D investment criteria to plan and assess programs and projects. The criteria were developed in 2001 and further refined with input from agencies, Congressional staff, the National Academy of Sciences, and numerous private sector and nonprofit stakeholders.

The chief elements of the R&D investment criteria are quality, relevance, and performance. Programs must demonstrate fulfillment of these elements. For example, to demonstrate relevance, programs are expected to have complete plans with clear goals and priorities. To demonstrate quality, programs are expected to commission periodic independent expert reviews. There are several other requirements, many of which R&D programs have and continue to undertake.

An additional set of criteria were established for R&D programs developing technologies that address industry issues. Some key elements of the criteria include: the ability of the programs to articulate the appropriateness and need for Federal assistance; relevance to the industry and the marketplace; identification of a transition point to industry commercialization (or of an off-ramp if progress does not meet expectations); and the potential public benefits, compared to alternative investments, that may accrue if the technology is successfully deployed.

The Office of Management and Budget (OMB)-Office of Science and Technology Policy (OSTP) guidance memorandum to agencies (http://www.ostp.gov/html/budget/2007/ostp_omb_guidancememo_FY07.pdf) describes the R&D investment criteria and identifies steps agencies should take to fulfill them. Where appropriate, throughout these justification materials, specific R&D investment criteria and requirements are cited to explain the Department's allocation of resources.

### Mission

SC's mission is to deliver the discoveries and scientific tools that transform our understanding of energy and matter and advance the national, economic, and energy security of the United States.

### Benefits

Developments at the nanoscale are expected to make major contributions to meeting DOE's applied mission needs such as strong, tough, ductile, lightweight materials with low failure rates that will improve the fuel efficiency and safety of ground and air transportation; smart materials that will range from paints that change color with temperature to windows that respond to thermal inputs and improve energy efficiency; nanostructured catalysts that will lead to cleaner, less expensive, more environmentally friendly petroleum refining; better batteries and fuel cells; improved chemical and product manufacturing; and innovative systems for harvesting light and storing energy that will dramatically improve solar energy conversion.

The knowledge developed from the Genomics: GTL program on understanding microbial genes and protein complexes, their regulation, and their functional roles in an ecosystem can lead both to greater energy security and a stabilization of net atmospheric $CO_2$ emissions. Currently, petroleum refineries "crack" raw oil through heat and catalysis to create gasoline and other petroleum products. In the future, we envision biorefineries that, in a one-step process, use microbial cellulase enzymes to crack the complex cellulose and hemicellulose in plant walls into simple sugars and microbially ferment those sugars into ethanol and other biobased products. Genomics: GTL research findings can accelerate this vision by improving the understanding of both plant cell-wall construction and the microbial enzymes necessary to deconstruct those walls. Microbes could also enable the inexpensive production of hydrogen by consuming a hydrogenated feedstock and releasing hydrogen. In addition, plants use the sun's energy to convert atmospheric carbon dioxide to biomass (e.g., leaves, roots, stems, and seeds) composed mainly of cellulose and lignin. Some biomass ultimately becomes incorporated into the soil where its carbon may be sequestered for hundreds of years. Understanding plant genes, their regulation and the role of microbes in the plant's root zone ultimately will enable manipulation of their carbon storage processes. Specialized, large-scale user facilities are needed to achieve the necessary economies of scale and output of molecular data associated with the Genomes: GTL effort.

Through investments in HEP and NP, SC has historically provided the Nation with fundamental knowledge about the laws of nature as they apply to the basic constituents of matter, and the forces between them. This knowledge rapidly travels from scientific journals to textbooks where it informs the creative vision of scientists, engineers, and entrepreneurs. This final path is neither linear nor overt, but we know that understanding the laws of nature is the key to technological progress. With this request, SC will focus efforts in these areas to places of world leadership and experiments with the greatest potential for radical discovery. The Relativistic Heavy Ion Collider (RHIC) will continue to explore new states of matter recently discovered there, providing a direct probe of the conditions found in exotic locations of the universe and at the first moments of the birth of the universe. Significant advances will be made in nuclear structure and nuclear astrophysics with the study of energy production in stars, the formation of heavy elements, and explosive stellar events. The Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) provides unique world-wide capabilities in polarized electron beam studies of the quark structure of the nucleon—it is the world's most powerful electron "microscope" for studying the nucleus with unprecedented resolving power. The Fermilab Tevatron, the world's highest energy accelerator, is turning its powerful beams to solve the mystery of the existence of mass, to find the first evidence of a supersymmetric universe, and to explore the distinct possibility of finding extra dimensions of space and time in which we live. The B-factory at the Stanford Linear Accelerator Center (SLAC) is providing precision measurements of how matter and antimatter behave differently in the decays of short-lived exotic particles known as B-mesons, considered by physicists to be vital to understanding why the whole universe appears to be predominantly matter, rather than an equal quantity of matter and antimatter. There is also a broad program of experiments that studies those aspects of the fundamental nature of particles, forces, and the universe that cannot be determined solely through the use of accelerators, including the search for or measurement of dark matter and dark energy. A recent example is the unexpected and significant finding that neutrinos have mass, discovered by studying solar and cosmic ray neutrinos.

**Strategic, General, and Program Goals**

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

Science Strategic Goal: To protect our national and economic security by providing world-class scientific research capacity and advancing scientific knowledge.

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

The programs funded by the Science appropriation have the following six Program Goals which contribute to General Goal 5 in the "goal cascade":

Program Goal 05.22.00.00: Advance the Basic Science for Energy Independence—Provide the scientific knowledge and tools to achieve energy independence, securing U.S. leadership and essential breakthroughs in basic energy sciences.

Program Goal 05.23.00.00: Deliver Computing for Accelerated Progress in Science—Deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.

Program Goal 05.21.00.00: Harness the Power of Our Living World—Provide the biological and environmental discoveries necessary to clean and protect our environment, offer new energy alternatives, and fundamentally change the nature of medical care to improve human health.

Program Goal 05.19.00.00: Explore the Fundamental Interactions of Energy, Matter, Time, and Space—Understand the unification of fundamental particles and forces and the mysterious forms of unseen energy and matter that dominate the universe, search for possible new dimensions of space, and investigate the nature of time itself.

Program Goal 05.20.00.00: Explore Nuclear Matter, from Quarks to Stars—Understand the evolution and structure of nuclear matter, from the smallest building blocks, quarks, and gluons; to the stable elements in the Universe created by stars; to unique isotopes created in the laboratory that exist at the limits of stability and possess radically different properties from known matter.

Program Goal 05.24.00.00: Bring the Power of the Stars to Earth—Answer the key scientific questions and overcome enormous technical challenges to harness the power that fuels our sun.

## Contribution to General Goals

Six of the programs within the Science appropriation directly contribute to General Goal 5 as follows:

BES contributes to General Goal 5 by advancing science through atomic- and molecular-level studies in materials sciences and engineering, chemistry, geosciences, and energy biosciences. BES also provides the Nation's researchers with world-class research facilities, including reactor and accelerator-based neutron sources, light sources including the X-ray free electron laser currently under construction, and micro-characterization centers. These facilities provide outstanding capabilities for imaging and characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological samples. Construction of the Spallation Neutron Source will be completed during the 3rd quarter of FY 2006 and will join the suite of BES scientific user facilities. Four Nanoscale Science Research Centers will begin their first full year of operation in FY 2007—the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, the Molecular Foundry at Lawrence Berkeley National Laboratory, the Center for Nanoscale Materials at Argonne National Laboratory, and the Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory. A fifth Center, the Center for Functional Nanomaterials at Brookhaven National Laboratory, will be in its final year of construction. The Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center is fully funded in FY 2007, including partial support for the SLAC linac. The Transmission Electron Aberration Corrected Microscope project continues as a Major Item of Equipment (MIE). Support is provided for R&D and project engineering and design (PED) activities for the National Synchrotron Light Source–II (NSLS–II) to enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. BES will increase support for basic research for the President's Hydrogen Fuel Initiative and will continue ongoing Scientific Discovery through Advanced Computing (SciDAC) efforts.

The ASCR program contributes to General Goal 5 by advancing mathematics and computer science, and developing the specialized algorithms, the scientific software tools, and the software libraries needed by DOE researchers to effectively use high-performance computing and networking hardware for scientific discovery. The ASCR program has been a leader in the computational sciences for several decades and has been acknowledged for pioneering accomplishments. The Leadership Computing activity will be expanded to Argonne National Laboratory to provide up to 100 teraflops of high performance computing capability with low electrical power needs to advance scientific understanding in areas that include materials science, biology, and advanced designs of nuclear reactors. The Leadership Computing

Facility at Oak Ridge National Laboratory will be upgraded to deliver 250 teraflops of peak capability in FY 2007. In FY 2007, the Energy Science Network (ESnet) will deliver a backbone network with two to four times the capability of today's network, to support the science mission of the Department. A procurement is planned in FY 2006 for the next generation of high performance resources at the National Energy Research Scientific Computing Center (NERSC) to be delivered in early FY 2007. This NERSC-5 system is expected to provide 100–150 teraflops of peak computing capacity. Corresponding investments in research and evaluation prototypes will help prepare scientists for petascale computing. ASCR will also continue core research efforts in applied mathematics and computer science and expand efforts in the SciDAC program and institutes.

BER contributes to General Goal 5 by advancing energy-related biological and environmental research in genomics and our understanding of complete biological systems, such as microbes that produce ethanol from cellulose or make hydrogen; by developing models to predict climate over decades to centuries; by developing science-based methods for cleaning up environmental contaminants; by providing regulators with a stronger scientific basis for developing future radiation protection standards; and by conducting limited research in medical imaging, radiopharmaceuticals, and development of an artificial retina. In FY 2007, BER will continue the Genomics: GTL program as a top priority, employing a systems approach to biology at the interface of the biological, physical, and computational sciences for DOE's energy security and environmental mission needs. Structural Biology infrastructure and innovative research on the biological effects of low dose radiation needed for future radiation protection standards will be sustained. BER continues as a pivotal partner in the interagency Climate Change Science Program focusing on the principal uncertainties of the causes and effects of climate change, the global carbon cycle, developing of predictive models for climate change over decades to centuries, and basic research for biological sequestration of carbon. Basic research in Environmental Remediation continues, at a reduced level, supporting fundamental research at the interfaces of biology, chemistry, geology, hydrology, and physics for solutions to environmental contamination challenges and terminating high level waste research. The Medical Sciences research program continues its principal focus on the artificial retina and medical imaging, including radiopharmaceuticals for imaging, at FY 2006 levels. Support for user facilities increases to meet growing scientific and technical demands for users of the Environmental Molecular Sciences Laboratory (EMSL), Production Genomics Facility (PGF), Atmospheric Radiation Measurement (ARM) sites, and Free Air Carbon Dioxide Enrichment (FACE) sites.

HEP contributes to General Goal 5 by advancing understanding of the basic constituents of matter, dark energy and dark matter, the lack of symmetry between matter and antimatter in the current universe, and the possible existence of other dimensions, collectively revealing key secrets of the universe. The FY 2007 budget request also contributes to this program goal by placing high priority on operations, upgrades, and infrastructure for the three major HEP user facilities (the Tevatron Collider and Neutrinos at the Main Injector [NuMI] at Fermilab and the B-factory at SLAC), to produce maximum scientific data. HEP and BES will jointly support accelerator operations at SLAC through the construction of the LCLS. The U.S. HEP program in FY 2007 will continue to lead the world with these forefront user facilities at Fermilab and SLAC, but these facilities will complete their scientific missions by the end of the decade. Thus the longer-term HEP program supported by this request begins to develop new cutting-edge facilities in targeted areas (for example, neutrino physics) that will establish U.S. leadership in these areas (see Significant Shifts) in the next decade, when the centerpiece of the world HEP program will reside at CERN. The FY 2007 budget also provides support for final installation, commissioning, and initial operations of the U.S.-supplied components of the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) Laboratory.

NP contributes to General Goal 5 by supporting innovative, peer-reviewed scientific research to advance knowledge and provide insights into the nature of energy and matter, and, in particular, to investigate the fundamental forces which hold the nucleus together and determine the detailed structure and behavior of the atomic nuclei. The program builds and supports world-leading scientific facilities and state-of-the-art instruments necessary to carry out its basic research agenda. NP also supports an effort in nuclear data that collects, evaluates, and disseminates nuclear physics data for basic nuclear research and for applied nuclear technologies, such as the design of reactors and national and homeland security. World-leading efforts on studies of hot dense nuclear matter and the origin of the proton spin with beams at the Relativistic Heavy Ion Collider (RHIC) will continue, including implementation of required instrumentation to realize scientific goals. A new Electron Beam Ion Source (EBIS) begins construction together with the National Aeronautics and Space Administration (NASA) to provide RHIC with more cost-effective, reliable operations. In addition to RHIC efforts, the High Energy Density Physics activities include NP contributions to enhance heavy ion capabilities of existing LHC experiments and the accompanying research program at universities and laboratories. Operations of the Continuous Electron Beam Accelerator Facility (CEBAF) are supported to provide high-energy electron beams to investigate a unique property called “confinement” that binds together the fundamental constituents of protons and neutrons, particles called quarks and gluons. At the FY 2007 level of funding, the accelerator provides beams simultaneously to all three experimental halls to better understand the structure of the nucleon. PED begins on a significant upgrade of the facility, the 12 GeV CEBAF Upgrade project. NP also continues efforts in nuclear structure/astrophysics, fundamental interactions, and neutrinos. Efforts at the Argonne Tandem Linear Accelerator System (ATLAS) and the Holifield Radioactive Ion Beam Facility (HRIBF) will be supported to focus on investigating new regions of nuclear structure, studying interactions in nuclear matter like those occurring in neutron stars, and determining the reactions that created the nuclei of the chemical elements inside stars and supernovae. Generic R&D in radioactive ion beam development, relevant for next-generation facilities in nuclear structure and astrophysics, is supported in FY 2007. The GRETINA gamma-ray tracking array, currently under fabrication, revolutionizes gamma ray detection technology and offers dramatically improved capabilities to study the structure of nuclei at ATLAS and HRIBF. The Fundamental Neutron Physics Beamline (FNPB) under fabrication at SNS will provide a world-class capability to study the neutron decay properties, leading to a refined characterization of the weak force. Investments are made to initiate the fabrication of a neutron Electric Dipole Moment experiment in the search for new physics beyond the Standard Model, for fabrication of instrumentation that will provide opportunities for U.S. involvement in the heavy-ion program at the CERN Large Hadron Collider, and for design and R&D associated with a Double Beta Decay experiment that will measure the absolute mass of the neutrino.

FES contributes to General Goal 5 by advancing the theoretical and experimental understanding of plasma and fusion science through our domestic activities and a close collaboration with international partners on specialized facilities abroad. FES also contributes to General Goal 5 through participation in ITER, an experiment to study and demonstrate the scientific and technical feasibility of fusion power. ITER is a multi-billion dollar international research project that will, if successful, advance progress towards developing fusion’s potential as a commercially viable and clean source of energy near the middle of the century. The FY 2006 Appropriation provided for a slower start for the U.S. Contributions to the ITER project. The FY 2007 request provides for the continuation of the U.S. Contributions to the ITER MIE project. In FY 2007, the overall Total Project Cost remains unchanged from FY 2006, but the funding requested in FY 2007 is lower than shown in the profile in the FY 2006 budget, and slightly adjusted between the Total Estimated Cost (TEC) and Other Project Cost (OPC) categories to address domestic and international project priorities. The U.S. contributions to the ITER project provides for the

U.S. “in-kind” equipment contributions, U.S. personnel to work at the ITER site, and cash for the U.S. share of common expenses such as infrastructure, hardware assembly, and installation.

Experimental research on tokamaks is continued in FY 2007, with increasing emphasis on physics issues of interest to the ITER project. Operations at the largest facility, the DIII-D tokamak at General Atomics (a private company), will increase from 7 weeks in FY 2006 to 12 weeks in FY 2007, while operations at C-Mod at MIT will increase from 14 to 15 weeks, and operations at the National Spherical Torus Experiment (NSTX) at PPPL will increase from 11 to 12 weeks. Fabrication of the National Compact Stellarator Experiment (NCSX) will continue along the new baseline established in July 2005 with completion expected in July 2009. The General Plasma Science program continues at approximately FY 2006 levels.

## Funding by General and Program Goal

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| General Goal 5, World-Class Scientific Research Capacity | | | |
| Program Goal 05.22.00.00, Basic Energy Sciences | 1,083,616 | 1,134,557 | 1,420,980 |
| Program Goal 05.23.00.00, Advanced Scientific Computing Research | 226,180 | 234,684 | 318,654 |
| Program Goal 05.21.00.00, Biological and Environmental Research | 566,597 | 579,831 | 510,263 |
| Program Goal 05.19.00.00, High Energy Physics | 722,906 | 716,694 | 775,099 |
| Program Goal 05.20.00.00, Nuclear Physics | 394,549 | 367,034 | 454,060 |
| Program Goal 05.24.00.00, Fusion Energy Sciences | 266,947 | 287,644 | 318,950 |
| Subtotal, General Goal 5, World-Class Scientific Research Capacity | 3,260,795 | 3,320,444 | 3,798,006 |
| All Other | | | |
| Science Laboratories Infrastructure | 37,498 | 41,684 | 50,888 |
| Program Direction | 154,031 | 159,118 | 170,877 |
| Workforce Development for Teachers and Scientists | 7,599 | 7,120 | 10,952 |
| Safeguards and Security | 72,773 | 73,630 | 76,592 |
| Small Business Innovation Research/Small Business Technology Transfer | 113,621 | —— | —— |
| Total, All Other | 385,622 | 281,552 | 309,309 |
| Total, General Goal 5 (Science) | 3,646,317 | 3,601,996 | 4,107,315 |

### Major FY 2005 Accomplishments

An incident solar photon striking a semiconductor solar cell normally produces a single electron-hole pair (exciton) and some excess heat. Experimentalists have recently demonstrated that two or more excitons can be created by absorption of a single photon in an array of lead-selenide nanocrystals. This process is called “impact ionization” and is observed when the photon energy is greater than three times the band gap of the nanocrystal. Multiple excitons from a single photon are formed on the picosecond time scale, and the process occurs with up to 100% efficiency depending on the excess energy of the absorbed photon. If this process could be translated into an operational solar cell, the gain in efficiency for converting light to electrical current would be greater than 35%.

Diatoms are simple single-celled algae, covered with elegant and often very beautiful casings sculpted from silica. They share biochemical features of both plants and animals and are related to the organisms that make up the well known White Cliffs of Dover in England. Scientists have taken a big step toward resolving the paradoxical nature of these odd microbes by sequencing the genome of the marine diatom *Thalassiosira pseudonana*. Analyses of these genes and the proteins they encode confirm that diatoms, in their evolutionary history, apparently acquired new genes by engulfing microbial neighbors including, possibly, genes that provided the diatom with all the machinery necessary for photosynthesis. Diatoms occupy vast swaths of ocean and fresh water, where they play a key role in the global carbon cycle. Diatom photosynthesis yields 19 billion tons of organic carbon—about 40% of the marine carbon produced each year—and thus represent one of nature's key defenses against global warming. Progress in analyzing the diatom genome is also shedding light on how a diatom constructs its intricately patterned glass shell, progress that could benefit both materials and climate change scientists.

The universe may have begun as a "perfect" liquid, not a gas. In April 2005, nuclear physicists working on the four experiments at RHIC presented "White Papers" documenting details and summarizing the evidence for an extraordinary new state of matter obtained from the first three years of RHIC operations. These latest results show that a new state of hot, dense matter was created out of quarks and gluons, but quite different and even more remarkable than had been previously predicted. The matter created in heavy-ion collisions appears to behave like a near "perfect" liquid rather than a fiery gas of free quarks and gluons. The word "perfect" refers to the liquid's viscosity—a friction like property that impedes a fluid's ability to flow. A perfect liquid has no viscosity. The RHIC results are consistent with "ideal" hydrodynamic calculations suggesting that the lowest viscosity possible in a "Quark-Gluon Plasma (QGP) fluid" may be achieved— a stunning discovery that could revise physicists' conception of the earliest moments of the universe.

**Program Assessment Rating Tool (PART)**

The Department implemented a tool to evaluate selected programs. PART was developed by the Office of Management and Budget (OMB) to provide a standardized way to assess the effectiveness of the Federal Government's portfolio of programs. The structured framework of the PART provides a means through which programs can assess their activities differently than through traditional reviews.

The current focus is to establish outcome- and output-oriented goals, the successful completion of which will lead to benefits to the public, such as increased national security and energy security, and improved environmental conditions. DOE has incorporated feedback from OMB into the FY 2006 Budget Request, and the Department will take the necessary steps to continue to improve performance.

SC did not complete PARTs for the FY 2007 Budget. In the FY 2005 PART review, OMB assessed six SC programs: ASCR, BES, BER, FES, HEP, and NP. Program scores ranged from 82-93%. Three programs—BES, BER, and NP—were assessed "Effective." Three programs—ASCR, FES, and HEP—were assessed "Moderately Effective." The full PARTs are available on the OMB website at http://www.whitehouse.gov/omb/budget/fy2005/part.html. SC expects to stagger updated PART reviews in the future.

SC has taken steps to enhance public understanding of our revised performance measures. The PART website (http://www.science.doe.gov/measures/) has been improved to better explain what each scientific measure means, why it is important to the Department and/or the research community, and how progress will be measured. Roadmaps with more detailed information on tracking progress toward the long-term measures have been developed with the Scientific Advisory Committees and are posted to this PART website. The Advisory Committees will review progress toward those measures vis-à-vis the roadmaps every three to five years. The first reviews will be conducted in FY 2006. The results of these reviews will be published on the PART website as they become available.

For the FY 2007 budget, OMB has developed PARTWeb—a new interface for PART that facilitates collaboration between agencies and OMB. PARTWeb will link to the new http://ExpectMore.gov website and will improve public access to PART assessments and follow up actions. New actions for Science in 2006 include:

- Implementing the recommendations of past and new external assessment panels, as appropriate;
- Engaging the Advanced Scientific Computing Advisory Committee and other outside groups in regular, thorough scientific assessments of the quality, relevance, and performance of its research portfolio and computing/network facilities;
- A detailed corporate solution for managing and operating the High Flux Isotope Reactor;
- Engaging the National Academies in an independent assessment of the scientific basis and business case for microbial genomics research efforts;
- Developing strategic and implementation plans in response to multiple Congressional requirements for ITER and Fusion Energy Sciences;
- Re-engaging the Fusion Energy Sciences Advisory Committee in a study of the how the program could best evolve over the coming decade to take into account new and upgraded international facilities;
- Developing a strategy and implementation plan for particle accelerator research and development, including a potential international linear collider;
- Engaging the National Academies to help develop a realistic long term plan for High Energy Physics that is based on prioritized scientific opportunities and input from across the scientific community;
- Engaging the National Academies, including experts outside of nuclear physics, to study the scientific capabilities of a proposed rare isotope accelerator in an international context; and
- Maximizing operational efficiency of major Nuclear Physics experimental facilities in response to increasing power costs.

**Significant Policy or Program Shifts**

Basic Energy Sciences—Over the next two to three years, the Spallation Neutron Source (SNS) will fabricate and commission instruments and increase power to full levels. A new major item of equipment is funded that will allow the fabrication of four to five additional instruments for the SNS, thus nearly completing the initial suite of twenty four instruments that can be accommodated in the high-power target station. BES also supports energy security through basic research for effective solar energy utilization, basic research for the hydrogen economy, and basic research underpinning advanced nuclear energy power.

Advanced Scientific Computing Research— In FY 2007, ASCR supports increases in SciDAC activities, the initiation of new university based competition for SciDAC Institutes, and enhancements to SciDAC that develop leadership class computing simulations for petaflop-scale computers. Increases in funding for both production and leadership computing facilities will enable continued scientific leadership through high performance computing. The success of this effort is built on the enhancements to the research and evaluation prototype and computer science research activities. The Research and Evaluation Prototypes activity will prepare users for the next generations of scientific computers and reduce the risk of major procurements. Increases in funding would also enable ESnet to evolve to manage the increased data flows from petascale computers and the experimental facilities that are critical to the Nation’s future.

Biological and Environmental Research—Development of a global biotechnology-based energy infrastructure requires a science base that enables scientists to redesign specific proteins, biochemical pathways, and even entire plants or microbes. Studies have suggested that, by 2100, biotechnology-based energy use could equal all global fossil energy use today. Two examples of biofuels are ethanol derived from the cellulose in plant cell walls (cellulosic ethanol) and hydrogen produced from water using energy from the sun (biophotolytic hydrogen). Within the Genomics: GTL program, BER will develop the understanding needed to advance biotechnology-based strategies for biofuel production. In addition, the FY 2007 budget includes funds for the continued expansion of the Genomics: GTL program—a program at the forefront of the biological revolution. Funding reductions are initiated in the Environmental Remediation Research and in the Climate Change Research Subprograms. High level waste, ocean sciences, and ocean carbon sequestration research are terminated within these two subprograms.

High Energy Physics—Our highest priority HEP R&D effort is the development of an International Linear Collider (ILC), and this request significantly advances the ILC R&D program. Pre-conceptual R&D for the ILC is doubled to enable a strong U.S. leadership role as a part of a comprehensive, coordinated international R&D program. In addition, R&D for other accelerator and detector technologies will continue at an increased level relative to FY 2006. Project engineering and design (PED) will begin on a new detector optimized to detect electron neutrinos, the Electron Neutrino Appearance (EνA) Detector, which will utilize the existing NuMI beam. Participation will begin in a reactor-based neutrino experiment, and R&D for a high-intensity neutrino super beam facility and a double beta decay experiment will continue. These efforts are part of a coordinated neutrino program developed from an American Physical Society study and a joint High Energy Physics Advisory Panel/Nuclear Science Advisory Committee review. In order to explore the nature of dark energy, conceptual R&D for the Super Nova/Acceleration Probe (SNAP) mission concept will continue in FY 2007. SNAP is expected to be a mission concept proposed for a potential interagency-sponsored experiment with NASA, the Joint Dark Energy Mission (JDEM). In addition, to fully determine the nature of dark energy, independent and complementary measurements are scientifically advisable. In FY 2007, additional R&D will be done for ground facilities and/or space-based facilities which could provide these measurements.

Nuclear Physics—The FY 2007 budget request increases support for operations and research by approximately 21% compared to FY 2006. At this level, operations of the four NP National User Facilities allow researchers to make effective progress towards the program's scientific goals and milestones. This budget request supports initiation of research efforts in the CERN LHC heavy ion program and starts PED activities for the 12 GeV CEBAF Upgrade project. NP also supports increases for research relevant to advanced nuclear fuel cycles. While we have a relatively good understanding of the origin of the chemical elements in the cosmos lighter than iron, the production of the elements from iron to uranium remains a puzzle. A next-generation exotic beam facility would allow the U.S. to play a leading role in nuclear structure and astrophysics studies in the next decade. Modest funding for generic R&D in exotic beam development is supported in FY 2007.

Fusion Energy Sciences—The FY 2007 budget continues the redirection of the fusion program to prepare for and participate in the international ITER project. The redirection will require modest reductions in several program elements not directly related to ITER. The FY 2007 request for the U.S. Contributions to ITER MIE project reflects a more modest first two years than was contained in the FY 2006 President's Budget, but maintains the overall Total Project Cost funding cap of $1,122,000,000. The reductions allow for the U.S. to be more consistent with the other ITER parties in the pace of starting the long lead procurements, in providing increased numbers of personnel to the ITER Organization, and in providing cash for common expenses. The profile is preliminary until the baseline scope, cost, and schedule for the MIE project are established, and the Director General Nominee and ITER Organization have achieved a standard mode of operation. SciDAC efforts will increase and will continue development of collaboratory tools to facilitate international fusion collaborations and initiate development of an integrated software environment that can accommodate the wide range of space and time scales and the multiple physical phenomena that are encountered in simulations of fusion systems. The Fusion Simulation Project is a major initiative involving plasma physicists, applied mathematicians, and computer scientists to create a comprehensive set of models of fusion systems, combined with the algorithms required to implement the models and the computational infrastructure to enable them to work together. High Energy Density Physics, Plasma Technology and Materials Research, Experimental Plasma Research, and Fusion Theory will be reduced.

Scientific Laboratory Infrastructure—In FY 2007, SLI will initiate funding for four construction projects: the Seismic Safety Upgrade of Buildings, Phase I, at the Lawrence Berkeley National Laboratory; the Modernization of Building 4500N, Wing 4, Phase I, at the Oak Ridge National Laboratory; the Building Electrical Services Upgrade, Phase II, at the Argonne National Laboratory; and Renovate Science Lab, Phase I, at the Brookhaven National Laboratory. Funding for the Pacific Northwest National Laboratory Physical Sciences Facility is requested in the National Nuclear Security Administration's (NNSA's) Nuclear Non-Proliferation R&D program for FY 2007. This project is co-funded by SC, NNSA, and the Department of Homeland Security. The SLI program will continue full funding for demolition of the Bevatron at Lawrence Berkeley National Laboratory. General plant project (GPP) funding is terminated in FY 2007 because it is supported in other SC programs' budgets in FY 2007.

Science Program Direction—Program direction funding increases by 7.4%, with most of the increase to support an additional 25 FTEs planned to be hired in support of the overall Science program, which is increased by 14.1% in the FY 2007 request. The increase also supports a 2.2% pay raise; an increased cap for SES basic pay; other pay related costs such as the government's contributions for employee health insurance and Federal Employees' Retirement System (FERS); escalation of non-pay categories, such as travel, training, and contracts; and increased e-Gov assessments and other fixed operating requirements across the SC complex. Finally, the increase will cover requirements not requested in previous SCPD budget requests, including travel expenses of SC Advisory Committee members and requirements related to Appendix A of OMB Circular A-123, Management's Responsibility for Internal Control.

Workforce Development for Teachers and Scientists—The Laboratory Science Teacher Professional Development (LSTPD) program increases to expand participation from 108 teachers in FY 2006 to 300 in FY 2007. The Faculty Sabbatical activity was initiated in FY 2005 for faculty from Minority Serving Institutions (MSI) and reduced in FY 2006 due to feedback from MSI faculty who expressed their inability to participate in sabbatical programs and a preference for shorter fellowship-type opportunities. FY 2007 participation will be reduced to two faculty members. The Science Undergraduate Laboratory Internship (SULI) programs will be increased to add approximately 55 students. The Albert Einstein Distinguished Educator Fellowship and the National and Middle School Science Bowls will all continue.

Safeguards and Security—The FY 2007 budget will ensure adequate security posture for SC facilities by protecting fundamental science, national security, and the health and safety of DOE and contractor employees, the public and the environment. FY 2007 funding will cover the implementation of the 2003 Design Basis Threat (DBT). In FY 2007, an increase in funding for the Cyber Security program element is being requested to begin to address the promulgation of new National Institute of Standards and Technology (NIST) requirements which are statutorily required by the Federal Information Security Management Act (FISMA) to improve the Federal and SC laboratory cyber security posture.

# Indirect Costs and Other Items of Interest

### Institutional General Plant Projects

Institutional General Plant Projects (IGPPs) are miscellaneous construction projects that are each less than $5,000,000 in TEC and are of a general nature (cannot be allocated to a specific program). IGPPs support multi-programmatic and/or inter-disciplinary programs and are funded through site overhead. Examples of acceptable IGPPs include site-wide maintenance facilities and utilities, such as roads and grounds outside the plant fences or a telephone switch that serves the entire facility.

Examples of current year projects are:

- Quadrangle Common Area design and construction at Oak Ridge National Laboratory. This FY 2004 and FY 2005 effort includes lawn, landscaping, sidewalks, lighting, and street improvements to an area of approximately 71,000 square feet. TEC: $2,697,000.
- East Campus Storm Water Upgrades at Oak Ridge National Laboratory. This FY 2005 project will upgrade the East Campus storm water drainage system to prevent flooding of new East Campus facilities. Recent storm modeling of the East Campus watershed has determined that a 500-year storm could produce substantial flooding in the Oak Ridge East Campus. TEC: $750,000
- East Campus Parking Expansion design and construction at Oak Ridge National Laboratory. This project, scheduled for completion in FY 2006, will provide expanded parking capacity for the recently completed Third Party Buildings, Joint Institute for Computational Science/Oak Ridge Center for Advanced Studies, and Research Support Center, as well as the Multiprogram Research Facility. TEC: $3,500,000.

The following displays IGPP funding by site:

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Oak Ridge National Laboratory | 9,000 | 10,000 | 8,000 |
| Pacific Northwest National Laboratory | 2,000 | 2,000 | 5,000 |
| Argonne National Laboratory | — | — | 2,000 |
| Total, IGPP | 11,000 | 12,000 | 15,000 |

# Facilities Maintenance and Repair

The Department's facilities maintenance and repair activities are tied to its programmatic missions, goals, and objectives. Facilities Maintenance and Repair activities funded by the Office of Science or at SC laboratories are displayed in the following tables. SC has set maintenance targets for each of its laboratories to achieve overall facilities maintenance and repair levels consistent with the National Academy of Science recommendation of 2%–4% of replacement plant value for the SC laboratory complex.

# Indirect-Funded Maintenance and Repair

Facilities maintenance and repair activities funded indirectly through overhead charges at SC laboratories are displayed below. Since this funding is allocated to all work done at each laboratory, these activities are paid for using funds from SC and other DOE organizations, as well other Federal agencies and other entities doing work at SC laboratories. Maintenance reported to SC for non-SC laboratories is also shown.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Ames Laboratory | 1,023 | 915 | 858 |
| Argonne National Laboratory | 26,413 | 26,327 | 28,332 |
| Brookhaven National Laboratory | 21,511 | 22,925 | 23,098 |
| Fermi National Accelerator Laboratory | 6,033 | 8,893 | 6,738 |
| Lawrence Berkeley National Laboratory | 11,175 | 13,000 | 15,440 |
| Lawrence Livermore National Laboratory | 2,735 | 2,767 | 2,822 |
| Massachusetts Institute of Technology | 569 | — | — |
| Oak Ridge Institute for Science and Education | 546 | 475 | 380 |
| Oak Ridge National Laboratory | 23,372 | 23,080 | 23,075 |
| Oak Ridge National Laboratory facilities at Y-12 | 738 | 500 | 500 |
| Pacific Northwest National Laboratory | 1,868 | 1,895 | 1,476 |
| Princeton Physics Plasma Laboratory | 4,387 | 5,045 | 5,300 |
| Sandia National Laboratory | 1,905 | 1,960 | 1,999 |
| Stanford Linear Accelerator Center | 5,837 | 5,278 | 5,140 |
| Thomas Jefferson National Accelerator Facility | 2,676 | 3,440 | 2,518 |
| Total, Indirect-Funded Maintenance and Repair | 110,788 | 116,500 | 117,676 |

## Direct-Funded Maintenance and Repair

Generally, facilities maintenance and repair expenses are funded through an indirect overhead charge. In some cases, however, a laboratory may charge maintenance directly to a specific program. An example of this might be if the maintenance were performed in a building used only by a single program. These direct-funded charges are nonetheless in the nature of indirect charges, and are not directly budgeted. The maintenance work for the Oak Ridge Office is direct funded and direct budgeted by the Science Laboratories Infrastructure program. A portion of the direct-funded maintenance and repair expenses reflects charges to non-SC programs performing work at SC laboratories.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Brookhaven National Laboratory | 2,290 | 2,974 | 2,974 |
| Fermilab National Accelerator Facility | 3,028 | 3,628 | 3,628 |
| Notre Dame Radiation Laboratory | 172 | 145 | 150 |
| Oak Ridge National Laboratory | 15,842 | 13,748 | 13,929 |
| Oak Ridge National Laboratory facilities at Y-12 | 79 | — | — |
| Oak Ridge Office | 1,771 | 1,891 | 2,019 |
| Stanford Linear Accelerator Center | 1,079 | 2,520 | 3,480 |
| Thomas Jefferson National Accelerator Facility | 44 | 50 | 52 |
| Total, Direct-Funded Maintenance and Repair | 24,305 | 24,956 | 26,232 |

## Deferred Maintenance Backlog Reduction

SC is planning an increased focus on reducing the backlog of deferred maintenance activities. SC will set targets for each of its laboratories for activities specifically focused on reduction of the backlog of these activities. The current deferred maintenance backlog at SC laboratories is estimated to be $660,000,000 and this amount will be our deferred maintenance baseline from which we will measure improvement. Deferred maintenance activities are primarily funded by the laboratories as overhead, charged to all uses of the laboratory facilities. The overall target for deferred maintenance at SC laboratories will be $19,800,000 in FY 2007. These deferred maintenance estimates are in addition to funding of day-to-day maintenance and repair amounts shown in the tables above. In order to assure that new maintenance requirements are not added to the backlog, SC has set targets for our laboratories that, overall, exceed 2% of the SC laboratory complex replacement plant value, commensurate with the industry standard funding level recommended by the National Academy of Sciences of 2–4% of the replacement plant value. The tables below show the targets planned for funding of deferred maintenance backlog reduction.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Argonne National Laboratory | — | — | 2,574 |
| Brookhaven National Laboratory | — | — | 5,940 |
| Fermi National Accelerator Laboratory | — | — | 1,980 |
| Lawrence Berkeley National Laboratory | — | — | 2,178 |
| Oak Ridge National Laboratory | — | — | 5,544 |
| Princeton Physics Plasma Laboratory | — | — | 396 |
| Stanford Linear Accelerator Center | — | — | 792 |
| Thomas Jefferson National Accelerator Facility | — | — | 396 |
| Total, Deferred Maintenance Backlog Reduction | — | — | 19,800 |

## Selected Administration Priorities

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Hydrogen Fuel Initiative | 29,183 | 32,500 | 50,000 |
| Climate Change Science Program | 126,985 | 130,646 | 126,187 |
| Networking and Information Technology Research and Development | 246,846 | 255,830 | 344,672 |
| National Nanotechnology Initiative | 207,837 | 206,404 | 256,914 |
| ITER (TPC) | —— | 19,315 | 60,000 |

# Science
# Office of Science
## Funding by Site by Program

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Ames Laboratory | | | |
| Basic Energy Sciences | 23,538 | 20,410 | 20,857 |
| Advanced Scientific Computing Research | 1,681 | 1,450 | 562 |
| Biological and Environmental Research | 800 | —— | —— |
| Science Laboratories Infrastructure | 210 | 150 | —— |
| Workforce Development for Teachers and Scientists | 65 | 65 | 227 |
| Safeguards and Security | 505 | 507 | 570 |
| Total, Ames Laboratory | 26,799 | 22,582 | 22,216 |
| Ames Site Office | | | |
| Science Program Direction | 470 | 453 | 520 |
| Argonne National Laboratory | | | |
| Basic Energy Sciences | 180,613 | 171,629 | 190,810 |
| Advanced Scientific Computing Research | 13,145 | 9,918 | 28,174 |
| Biological and Environmental Research | 26,291 | 27,297 | 27,713 |
| High Energy Physics | 10,829 | 8,939 | 9,748 |
| Nuclear Physics | 23,158 | 18,762 | 23,682 |
| Fusion Energy Sciences | 971 | 990 | 960 |
| Science Laboratories Infrastructure | 2,457 | 1,246 | 3,697 |
| Workforce Development for Teachers and Scientists | 1,833 | 298 | 2,056 |
| Safeguards and Security | 8,671 | 8,570 | 8,462 |
| Total, Argonne National Laboratory | 267,968 | 247,649 | 295,302 |
| Argonne Site Office | | | |
| Science Program Direction | 3,413 | 3,677 | 3,813 |
| Berkeley Site Office | | | |
| Science Program Direction | 3,361 | 3,675 | 4,241 |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Brookhaven National Laboratory | | | |
| Basic Energy Sciences | 89,876 | 101,633 | 133,783 |
| Advanced Scientific Computing Research | 1,000 | 673 | —— |
| Biological and Environmental Research | 23,620 | 20,172 | 18,074 |
| High Energy Physics | 30,648 | 26,542 | 30,193 |
| Nuclear Physics | 158,441 | 146,832 | 183,255 |
| Science Laboratories Infrastructure | 7,706 | 4,996 | 5,100 |
| Workforce Development for Teachers and Scientists | 734 | 436 | 1,013 |
| Safeguards and Security | 11,335 | 11,229 | 10,967 |
| Total, Brookhaven National Laboratory | 323,360 | 312,513 | 382,385 |
| | | | |
| Brookhaven Site Office | | | |
| Science Program Direction | 3,267 | 3,537 | 3,643 |
| | | | |
| Chicago Office | | | |
| Basic Energy Sciences | 180,295 | 130,276 | 130,351 |
| Advanced Scientific Computing Research | 41,556 | 24,853 | 18,164 |
| Biological and Environmental Research | 220,252 | 109,654 | 75,868 |
| High Energy Physics | 127,944 | 117,772 | 120,152 |
| Nuclear Physics | 73,339 | 59,258 | 61,664 |
| Fusion Energy Sciences | 135,356 | 134,241 | 129,817 |
| Science Laboratories Infrastructure | 1,848 | —— | 1,520 |
| Science Program Direction | 25,306 | 24,719 | 26,162 |
| Workforce Development for Teachers and Scientists | 36 | —— | —— |
| Safeguards and Security | 185 | 825 | 3,400 |
| SBIR/STTR | 113,621 | —— | —— |
| Total, Chicago Office | 919,738 | 601,598 | 567,098 |
| | | | |
| Fermi National Accelerator Laboratory | | | |
| Advanced Scientific Computing Research | 646 | 1,215 | —— |
| High Energy Physics | 318,316 | 298,533 | 320,367 |
| Nuclear Physics | 33 | —— | —— |
| Fusion Energy Sciences | —— | 3 | —— |
| Science Laboratories Infrastructure | 662 | 491 | —— |
| Workforce Development for Teachers and Scientists | 62 | 50 | 308 |
| Safeguards and Security | 3,015 | 2,893 | 3,221 |
| Total, Fermi National Accelerator Laboratory | 322,734 | 303,185 | 323,896 |

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| | (dollars in thousands) | | |
| Fermi Site Office | | | |
| Science Program Direction | 2,185 | 2,235 | 2,346 |
| Golden Field Office | | | |
| Basic Energy Sciences | —— | 4 | 4 |
| Advanced Scientific Computing Research | —— | 3 | —— |
| Biological and Environmental Research | —— | 3 | —— |
| High Energy Physics | —— | 4 | —— |
| Nuclear Physics | —— | 3 | —— |
| Workforce Development for Teachers and Scientists | 622 | 250 | 835 |
| Total, Golden Field Office | 622 | 267 | 839 |
| Idaho National Laboratory | | | |
| Basic Energy Sciences | 353 | 225 | 225 |
| Biological and Environmental Research | 3,670 | 1,566 | 1,190 |
| Fusion Energy Sciences | 2,499 | 2,380 | 2,334 |
| Workforce Development for Teachers and Scientists | 75 | 70 | 340 |
| Total, Idaho National Laboratory | 6,597 | 4,241 | 4,089 |
| Idaho Operations Office | | | |
| Biological and Environmental Research | 1,113 | —— | —— |
| Lawrence Berkeley National Laboratory | | | |
| Basic Energy Sciences | 135,564 | 110,437 | 125,497 |
| Advanced Scientific Computing Research | 71,546 | 65,408 | 77,559 |
| Biological and Environmental Research | 71,818 | 71,517 | 72,671 |
| High Energy Physics | 43,101 | 40,834 | 44,812 |
| Nuclear Physics | 18,784 | 18,399 | 20,706 |
| Fusion Energy Sciences | 6,048 | 5,653 | 4,911 |
| Science Laboratories Infrastructure | 8,199 | 15,009 | 21,500 |
| Workforce Development for Teachers and Scientists | 799 | 379 | 885 |
| Safeguards and Security | 5,733 | 4,723 | 4,981 |
| Total, Lawrence Berkeley National Laboratory | 361,592 | 332,359 | 373,522 |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Lawrence Livermore National Laboratory | | | |
| Basic Energy Sciences | 3,405 | 2,819 | 2,854 |
| Advanced Scientific Computing Research | 6,734 | 4,743 | 1,800 |
| Biological and Environmental Research | 26,149 | 24,224 | 25,209 |
| High Energy Physics | 2,140 | 1,951 | 2,196 |
| Nuclear Physics | 1,084 | 643 | 905 |
| Fusion Energy Sciences | 13,751 | 13,282 | 12,025 |
| Science Laboratories Infrastructure | 150 | 150 | —— |
| Workforce Development for Teachers and Scientists | 50 | —— | 78 |
| Total, Lawrence Livermore National Laboratory | 53,463 | 47,812 | 45,067 |
| | | | |
| Los Alamos National Laboratory | | | |
| Basic Energy Sciences | 27,624 | 22,753 | 21,993 |
| Advanced Scientific Computing Research | 3,879 | 2,832 | 2,075 |
| Biological and Environmental Research | 20,825 | 17,675 | 15,479 |
| High Energy Physics | 809 | 540 | 590 |
| Nuclear Physics | 9,647 | 8,008 | 10,515 |
| Fusion Energy Sciences | 3,831 | 3,946 | 3,356 |
| Workforce Development for Teachers and Scientists | 50 | 50 | 361 |
| Total, Los Alamos National Laboratory | 66,665 | 55,804 | 54,369 |
| | | | |
| National Energy Technology Laboratory | | | |
| Basic Energy Sciences | 82 | 100 | —— |
| Biological and Environmental Research | 31 | —— | —— |
| High Energy Physics | 81 | —— | —— |
| Nuclear Physics | 16 | 100 | —— |
| Fusion Energy Sciences | 81 | 3 | —— |
| Science Laboratories Infrastructure | —— | 275 | —— |
| Workforce Development for Teachers and Scientists | 127 | 263 | 500 |
| Total, National Energy Technology Laboratory | 418 | 741 | 500 |
| | | | |
| National Renewable Energy Laboratory | | | |
| Basic Energy Sciences | 8,043 | 7,197 | 7,403 |
| Advanced Scientific Computing Research | 150 | 150 | 150 |
| Biological and Environmental Research | 400 | 569 | 875 |
| Workforce Development for Teachers and Scientists | 52 | —— | —— |
| Total, National Renewable Energy Laboratory | 8,645 | 7,916 | 8,428 |
| | | | |
| NNSA Service Center/Albuquerque | | | |
| Biological and Environmental Research | 850 | 800 | —— |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Oak Ridge Institute for Science and Education | | | |
| Basic Energy Sciences | 3,455 | 810 | 810 |
| Advanced Scientific Computing Research | 315 | 600 | —— |
| Biological and Environmental Research | 5,557 | 4,088 | 4,159 |
| High Energy Physics | 278 | 50 | —— |
| Nuclear Physics | 1,067 | 590 | 703 |
| Fusion Energy Sciences | 1,186 | 1,215 | 788 |
| Science Laboratories Infrastructure | 565 | 768 | —— |
| Science Program Direction | 39 | —— | —— |
| Workforce Development for Teachers and Scientists | 1,470 | 853 | 1,545 |
| Safeguards and Security | 1,403 | 1,359 | 1,489 |
| Total, Oak Ridge Institute for Science and Education | 15,335 | 10,333 | 9,494 |
| Oak Ridge National Laboratory | | | |
| Basic Energy Sciences | 263,802 | 276,351 | 322,480 |
| Advanced Scientific Computing Research | 68,786 | 61,098 | 82,822 |
| Biological and Environmental Research | 45,408 | 39,746 | 36,266 |
| High Energy Physics | 836 | 180 | 182 |
| Nuclear Physics | 20,941 | 19,668 | 23,349 |
| Fusion Energy Sciences | 22,340 | 20,560 | 18,650 |
| Science Laboratories Infrastructure | 2,188 | 1,283 | 8,047 |
| Safeguards and Security | 11,891 | 9,461 | 8,396 |
| Total, Oak Ridge National Laboratory | 436,192 | 428,347 | 500,192 |
| Oak Ridge Office | | | |
| Basic Energy Sciences | 106 | 80 | 80 |
| Advanced Scientific Computing Research | 200 | 80 | —— |
| Biological and Environmental Research | 694 | 677 | 373 |
| High Energy Physics | 108 | 16 | 80 |
| Nuclear Physics | 106 | 80 | —— |
| Fusion Energy Sciences | 106 | 80 | —— |
| Science Laboratories Infrastructure | 5,039 | 5,028 | 5,079 |
| Science Program Direction | 42,422 | 42,534 | 44,252 |
| Workforce Development for Teachers and Scientists | 90 | 90 | 90 |
| Safeguards and Security | 12,862 | 16,107 | 17,975 |
| Total, Oak Ridge Office | 61,733 | 64,772 | 67,929 |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Pacific Northwest National Laboratory | | | |
| Basic Energy Sciences | 15,149 | 14,763 | 15,182 |
| Advanced Scientific Computing Research | 3,408 | 6,690 | 350 |
| Biological and Environmental Research | 86,647 | 80,203 | 85,695 |
| Fusion Energy Sciences | 1,330 | 1,285 | 815 |
| Science Laboratories Infrastructure | 4,960 | 4,950 | — |
| Workforce Development for Teachers and Scientists | 917 | 514 | 1,035 |
| Safeguards and Security | 11,133 | 10,044 | 10,993 |
| Total, Pacific Northwest National Laboratory | 123,544 | 118,449 | 114,070 |
| | | | |
| Pacific Northwest Site Office | | | |
| Science Program Direction | 5,277 | 5,438 | 5,553 |
| | | | |
| Princeton Plasma Physics Laboratory | | | |
| Advanced Scientific Computing Research | 573 | 1,143 | — |
| High Energy Physics | 225 | 225 | 249 |
| Fusion Energy Sciences | 74,999 | 90,953 | 129,956 |
| Science Laboratories Infrastructure | 239 | 119 | — |
| Workforce Development for Teachers and Scientists | 135 | 115 | 392 |
| Safeguards and Security | 1,938 | 1,819 | 1,953 |
| Total, Princeton Plasma Physics Laboratory | 78,109 | 94,374 | 132,550 |
| | | | |
| Princeton Site Office | | | |
| Science Program Direction | 1,554 | 1,618 | 1,668 |
| | | | |
| Sandia National Laboratories | | | |
| Basic Energy Sciences | 54,225 | 38,808 | 43,822 |
| Advanced Scientific Computing Research | 10,693 | 4,122 | 2,595 |
| Biological and Environmental Research | 7,125 | 4,631 | 4,213 |
| Fusion Energy Sciences | 3,454 | 2,022 | 1,655 |
| Workforce Development for Teachers and Scientists | — | — | 258 |
| Total, Sandia National Laboratories | 75,497 | 49,583 | 52,543 |
| | | | |
| Savannah River National Laboratory | | | |
| Basic Energy Sciences | 200 | 200 | 200 |
| Biological and Environmental Research | 873 | 804 | 691 |
| Fusion Energy Sciences | 37 | 10 | — |
| Workforce Development for Teachers and Scientists | — | — | 258 |
| Total, Savannah River National Laboratory | 1,110 | 1,014 | 1,149 |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Savannah River Operations Office | | | |
| Biological and Environmental Research | 7,748 | 1,000 | —— |
| | | | |
| Stanford Linear Accelerator Center | | | |
| Basic Energy Sciences | 95,232 | 150,763 | 215,469 |
| Advanced Scientific Computing Research | 485 | 57 | —— |
| Biological and Environmental Research | 4,150 | 4,350 | 4,311 |
| High Energy Physics | 169,036 | 144,574 | 145,964 |
| Science Laboratories Infrastructure | 3,275 | 5,539 | 5,770 |
| Workforce Development for Teachers and Scientists | 150 | 135 | 150 |
| Safeguards and Security | 2,335 | 2,377 | 2,437 |
| Total, Stanford Linear Accelerator Center | 274,663 | 307,795 | 374,101 |
| | | | |
| Stanford Site Office | | | |
| Science Program Direction | 1,647 | 1,670 | 2,134 |
| | | | |
| Thomas Jefferson National Accelerator Facility | | | |
| Advanced Scientific Computing Research | 50 | —— | —— |
| Biological and Environmental Research | 810 | 400 | 400 |
| High Energy Physics | 50 | 480 | 927 |
| Nuclear Physics | 86,815 | 78,127 | 96,371 |
| Science Laboratories Infrastructure | —— | 175 | —— |
| Workforce Development for Teachers and Scientists | 332 | 95 | 502 |
| Safeguards and Security | 1,468 | 1,231 | 1,311 |
| Total, Thomas Jefferson National Accelerator Facility | 89,525 | 80,508 | 99,511 |
| | | | |
| Thomas Jefferson Site Office | | | |
| Science Program Direction | 1,407 | 1,457 | 1,500 |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Washington Headquarters | | | |
| Basic Energy Sciences | 2,054 | 85,299 | 189,160 |
| Advanced Scientific Computing Research | 1,333 | 49,649 | 104,403 |
| Biological and Environmental Research | 11,766 | 170,455 | 137,076 |
| High Energy Physics | 18,505 | 76,054 | 99,639 |
| Nuclear Physics | 1,118 | 16,564 | 32,910 |
| Fusion Energy Sciences | 958 | 11,021 | 13,683 |
| Science Laboratories Infrastructure | — | 1,505 | 175 |
| Science Program Direction | 63,683 | 68,105 | 75,045 |
| Workforce Development for Teachers and Scientists | — | 3,457 | 119 |
| Safeguards and Security | 299 | 2,485 | 437 |
| Total, Washington Headquarters | 99,716 | 484,594 | 652,647 |
| Total, Science | 3,646,317 | 3,601,996 | 4,107,315 |

# Major Changes or Shifts by Site

## Argonne National Laboratory

### Basic Energy Sciences

- The **Center for Nanoscale Materials**, one of five DOE Nanoscale Science Research Centers, will be fully operational in FY 2007.

### Advanced Scientific Computing Research

- The Leadership Computing activity will be initiated to provide up to 100 teraflops of high-performance computing capability with low electrical power consumption to enable scientific advances.

### Science Laboratories Infrastructure

- The Argonne National Laboratory (ANL) Building Electrical Services Upgrade, Phase II project is initiated to upgrade critical portions of the electrical power distribution system in twelve research buildings and support facilities, including the Canal Water Plant supplying cooling water for site experiments.

## Lawrence Berkeley National Laboratory

### Basic Energy Sciences

- The Molecular Foundry, one of five DOE Nanoscale Science Research Centers, will be fully operational in FY 2007.
- Advanced Light Source (ALS) User Support Building (USB) will begin design in FY 2007. The USB will provide user support space to accommodate the growth in the number of users and future expansion of the ALS.

**Advanced Scientific Computing Research**

- Funding for the National Energy Research Scientific Computing Center (NERSC) and the Energy Science Network (ESnet) is increased from FY 2006. This will enable significant increases in the high performance production computing capacity and network capacity to meet SC's needs.

**Science Laboratories Infrastructure**

- The Seismic Safety Upgrade of Buildings, Phase I project is initiated to address the seismic upgrade of laboratory buildings where high life-safety risks have been identified.
- Demolition of the Bevatron is fully funded to free-up about 7.5% of the total building space for future missions.

**Brookhaven National Laboratory**

**Basic Energy Sciences**

- The **Center for Functional Nanomaterials**, one of five DOE Nanoscale Science Research Centers, is in its final year of construction in FY 2007.
- Support is provided for Project Engineering Design and Other Project Costs for the **National Synchrotron Light Source-II** (NSLS-II), which will be built as a replacement for NSLS-I, to enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. NSLS-II will provide the world's finest capabilities for x-ray imaging.

**Science Laboratories Infrastructure**

- The Renovate Science Laboratory, Phase I project is initiated to upgrade and rehabilitate existing obsolete and unsuitable laboratory facilities into modern, efficient facilities compatible with world-class scientific research.

**Los Alamos National Laboratory**

**Basic Energy Sciences**

- The **Center for Integrated Nanotechnologies**, one of five DOE Nanoscale Science Research Centers, will be fully operational in FY 2007.

**Oak Ridge National Laboratory**

**Basic Energy Sciences**

- Construction of the **Spallation Neutron Source** (SNS) will be completed during the 3rd quarter of FY 2006. Over the next two to three years, the facility will continue to fabricate and commission instruments, funded both as part of the SNS project and from other sources including non-DOE sources, and will increase power to full levels. A new Major Item of Equipment is funded in FY 2007 that will allow the fabrication of approximately four to five additional instruments for the SNS, thus nearly completing the initial suite of 24 instruments that can be accommodated in the high-power target station. Support also is provided for research and development (R&D) for a power upgrade to the SNS.
- The **Center for Nanophase Materials Sciences**, one of five DOE Nanoscale Science Research Centers, will be fully operational in FY 2007.

**Advanced Scientific Computing Research**

- The Leadership Computing Facility (LCF) at the Oak Ridge National Laboratory (ORNL) will be enhanced to deliver 250 teraflops of peak capability in FY 2007 for scientific applications.

**Fusion Energy Sciences**

- ORNL, in partnership with Princeton Plasma Physics Laboratory (PPPL), shares the responsibility for managing the U.S. contributions to the ITER project by further engaging the U.S. fusion community and industry to provide the U.S. hardware contributions and the U.S. secondees to be assigned to the ITER Organization abroad. There will be significant international cooperation between the U.S. ITER Project Office (a partnership between PPPL and ORNL), the international ITER Organization, and the other ITER parties.

**Science Laboratories Infrastructure**

- The Modernization of Building 4500N, Wing 4, Phase I, project is initiated to rehabilitate a facility housing many of the laboratory's chemical laboratory facilities, as well as administrative offices and the medical clinic.

**Princeton Plasma Physics Laboratory**

**Fusion Energy Sciences**

- PPPL, in partnership with ORNL, will continue to manage the U.S. contributions to the ITER project by further engaging the U.S. fusion community and industry to provide the U.S. hardware contributions and the U.S. secondees to be assigned to the ITER Organization abroad. There will be significant international cooperation and coordination between the U.S. ITER Project Office (a partnership between PPPL and ORNL), the international ITER Organization, and the other ITER parties.

**Sandia National Laboratories**

**Basic Energy Sciences**

- The **Center for Integrated Nanotechnologies**, one of five DOE Nanoscale Science Research Centers, will be fully operational in FY 2007.

**Fusion Energy Sciences**

- Research in plasma-facing components and plasma materials interactions for the base program will be reduced; however, Sandia is expected to play a major role in the first wall and shield area of the ITER project.

**Stanford Linear Accelerator Center**

**Basic Energy Sciences**

- The **Linac Coherent Light Source (LCLS)** will continue Project Engineering Design and construction. Funding is provided separately for preconceptual design and fabrication of instruments for the facility. Funding is also provided to partially support operation of the SLAC linac. This marks the second year of the transition to LCLS operations at SLAC.

## Site Description

### Ames Laboratory

#### Introduction

The Ames Laboratory is a program dedicated laboratory (Basic Energy Sciences). The laboratory is located on the campus of the Iowa State University, in Ames, Iowa, and consists of 12 buildings (327,664 gross square feet of space) with the average age of the buildings being 37 years. DOE does not own the land. Ames conducts fundamental research in the physical, chemical, and mathematical sciences associated with energy generation and storage and is a national center for the synthesis, analysis, and engineering of rare-earth metals and their compounds.

#### Basic Energy Sciences

Ames supports experimental and theoretical research on rare earth elements in novel mechanical, magnetic, and superconducting materials. Ames scientists are experts on magnets, superconductors, and quasicrystals that incorporate rare earth elements. Ames also supports theoretical studies for the prediction of molecular energetics and chemical reaction rates and provides leadership in analytical and separations chemistry.

Ames is home to the **Materials Preparation Center (MPC)**, which is dedicated to the preparation, purification, and characterization of rare-earth, alkaline-earth, and refractory metal and oxide materials. Established in 1981, the MPC is a one-of-a-kind resource that provides scientists at university, industrial, and government laboratories with research and developmental quantities of high purity materials and unique analytical and characterization services that are not available from commercial suppliers. The MPC is renowned for its technical expertise in alloy design and for creating materials that exhibit ultrafine microstructures, high strength, magnetism, and high conductivity.

#### Advanced Scientific Computing Research

Ames conducts research in computer science and participates on SciDAC teams. Ames also participates in Integrated Software Infrastructure Center (ISIC) activities that focus on specific software challenges confronting users of terascale computers.

#### Science Laboratories Infrastructure

The Science Laboratories Infrastructure (SLI) program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

#### Safeguards and Security

This program coordinates planning, policy, implementation, and oversight in the areas of security systems, protective forces, personnel security, program management, material control and accountability, and cyber security. A protective force is maintained to provide protection of personnel, equipment, and property from acts of theft, vandalism, and sabotage through facility walk-through, monitoring of electronic alarm systems, and emergency communications.

### Ames Site Office

#### Introduction

The Ames Site Office provides the single federal presence with responsibility for contract performance at the Ames Laboratory. This site office provides an on-site Office of Science (SC) presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

### Argonne National Laboratory

#### Introduction

The Argonne National Laboratory (ANL) in Argonne, Illinois, is a multiprogram laboratory located on 1,508 acres in suburban Chicago. The laboratory consists of 99 buildings (4.5 million gross square feet of space) with an average building age of 34 years.

#### Basic Energy Sciences

ANL is home to research activities in broad areas of materials and chemical sciences. It is also the site of four user facilities—the Advanced Photon Source (APS), the Intense Pulsed Neutron Source (IPNS), the Center for Nanoscale Materials (CNM), and the Electron Microscopy Center (EMC) for Materials Research.

The **Advanced Photon Source** is one of only three third-generation, hard x-ray synchrotron radiation light sources in the world. The 1,104-meter circumference facility—large enough to house a baseball park in its center—includes 34 bending magnets and 34 insertion devices, which generate a capacity of 68 beamlines for experimental research. Instruments on these beamlines attract researchers to study the structure and properties of materials in a variety of disciplines, including condensed matter physics, materials sciences, chemistry, geosciences, structural biology, medical imaging, and environmental sciences. The high-quality, reliable x-ray beams at the APS have already brought about new discoveries in materials structure.

The **Intense Pulsed Neutron Source** is a short-pulsed spallation neutron source that first operated all of its instruments in the user mode in 1981. Twelve neutron beam lines serve 14 instruments. Distinguishing characteristics of IPNS include its innovative instrumentation and source technology and its dedication to serving the users. The first generation of virtually every pulsed source neutron scattering instrument was developed at IPNS. In addition, the source and moderator technologies developed at IPNS, including uranium targets, liquid hydrogen and methane moderators, solid methane moderators, and decoupled reflectors, have impacted spallation sources worldwide. Research at IPNS is conducted on the structure of high-temperature superconductors, alloys, composites, polymers, catalysts, liquids and non-crystalline materials, materials for advanced energy technologies, and biological materials.

The **Electron Microscopy Center for Materials Research** provides *in-situ*, high-voltage and intermediate voltage, high-spatial resolution electron microscope capabilities for direct observation of ion-solid interactions during irradiation of samples with high-energy ion beams. The EMC employs both a tandem accelerator and an ion implanter in conjunction with a transmission electron microscope for simultaneous ion irradiation and electron beam microcharacterization. It is the only instrumentation of its type in the western hemisphere. The unique combination of two ion accelerators and an electron microscope permits direct, real-time, *in-situ* observation of the effects of ion bombardment of materials and consequently attracts users from around the world. Research at EMC includes microscopy based studies on high-temperature superconducting materials, irradiation effects in metals and semiconductors, phase transformations, and processing related structure and chemistry of interfaces in thin films.

The **Center for Nanoscale Materials** provides capabilities for developing new methods for self assembly of nanostructures, exploring the nanoscale physics and chemistry of nontraditional electronic materials, and creating new probes for exploring nanoscale phenomena. The CNM is organized around six scientific themes: nanomagnetism, bio-inorganic hybrids, nanocarbon, complex oxides, nanophotonics, and theory and simulation.

**Advanced Scientific Computing Research**

ANL conducts basic research in mathematics and computer science, as well as research in advanced computing software tools. ANL also participates in scientific application partnerships and participates on a number of the SciDAC teams. Further, it participates in ISIC activities that focus on specific software challenges confronting users of terascale computers. As part of the Leadership Computing Facility (LCF) activity, ANL will acquire up to 100 teraflops of high-performance computing with low electrical power consumption to advance science and will continue to focus on testing and evaluating leading edge computers.

**Biological and Environmental Research**

ANL operates a high-throughput national user facility for protein crystallography at APS that also supports a growing environmental science community. In support of climate change research, it coordinates the operation and development of the Southern Great Plains, Tropical Western Pacific, and North Slope of Alaska Atmospheric Radiation Measurement (ARM) sites. ANL also conducts research on aerosol processes and properties and to develop and apply software to enable efficient long-term climate simulations on distributed-memory multiprocessor computing platforms. Research is conducted to understand the molecular control of genes and gene pathways in microbes. In conjunction with the ORNL and the Pacific Northwest National Laboratory (PNNL) and six universities, ANL is a participating lab in the Carbon Sequestration in Terrestrial Ecosystems (CSiTE) consortium, focusing on research to understand the processes controlling the rate of soil carbon accretion. APS supports environmental remediation sciences researchers and ANL conducts environmental remediation sciences research.

**High Energy Physics**

The High Energy Physics (HEP) program supports physics research and technology R&D at ANL, using unique capabilities of the laboratory in the areas of engineering and detector technology and advanced accelerator and computing techniques.

**Nuclear Physics**

The major ANL activity is the operation and R&D program at the Argonne Tandem Linac Accelerator System (ATLAS) National User Facility. Other activities include an on-site program of research using laser techniques (Atom Trap Trace Analysis); research programs at the Thomas Jefferson National Accelerator Facility (TJNAF), Fermi National Laboratory (Fermilab), Relativistic Heavy Ion Collider (RHIC), and DESY in Germany investigating the structure of the nucleon; generic R&D in rare isotope beam development relevant for a next generation facility in nuclear structure and astrophysics, such as the proposed Rare Isotope Accelerator (RIA) facility; theoretical calculations and investigations in subjects supporting the experimental research programs in Medium Energy and Low Energy physics; and data compilation and evaluation activities as part of the National Nuclear Data Program.

The **Argonne Tandem Linac Accelerator System** facility provides variable energy, precision beams of stable ions from protons through uranium, at energies near the Coulomb barrier (up to 10 MeV per nucleon) using a superconducting linear accelerator. Most work is performed with stable heavy-ion beams; however, about 10% of the beams are exotic (radioactive) beams. The ATLAS facility features a wide array of experimental instrumentation, including a world-leading ion-trap apparatus, the Advanced Penning Trap. The Gammasphere detector, coupled with the Fragment Mass Analyzer, is a unique world facility for measurement of nuclei at the limits of angular momentum (high-spin states). ATLAS staff are world leaders in superconducting linear accelerator technology, with particular application in exotic beam facilities. The combination of versatile beams and powerful instruments enables ~200 users annually at ATLAS to conduct research in a broad program in nuclear structure and dynamics, nuclear astrophysics, and fundamental interaction studies. The capabilities of ATLAS are being augmented by the fabrication of a Californium source to provide new capabilities in neutron-rich radioactive beams.

**Fusion Energy Sciences**

Argonne contributes to the plasma facing components area of the enabling R&D program activities, focusing on modeling of plasma-materials interaction phenomena of interest for ITER and current plasma experiments.

**Science Laboratories Infrastructure**

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

**Safeguards and Security**

This program provides protection of nuclear materials, classified matter, government property, and other vital assets from unauthorized access, theft, diversion, sabotage, espionage, and other hostile acts that may cause risks to national security, the health and safety of DOE and contractor employees, the public, or the environment. Program activities include security systems, material control and accountability, information and cyber security, program management, and personnel security. In addition, a protective force is maintained. These activities ensure that the facility, personnel, and assets remain safe from potential threats.

## Argonne Site Office

### Introduction

The Argonne Site Office provides the single federal presence with responsibility for contract performance at the Argonne National Laboratory (ANL). This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Berkeley Site Office

### Introduction

The Berkeley Site Office provides the single federal presence with responsibility for contract performance at the Lawrence Berkeley National Laboratory (LBNL). This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Brookhaven National Laboratory

### Introduction

The Brookhaven National Laboratory is a multiprogram laboratory located on 5,300 acres in Upton, New York. The laboratory consists of 345 SC buildings (3.9 million gross square feet of space) with an average building age of 36 years. BNL creates and operates major facilities available to university, industrial, and government personnel for basic and applied research in the physical, biomedical, and environmental sciences, and in selected energy technologies.

### Basic Energy Sciences

BNL conducts research efforts in materials and chemical sciences as well as to efforts in geosciences and biosciences. It is also the site of one BES supported user facilities—the National Synchrotron Light Source (NSLS).The **National Synchrotron Light Source** is among the largest and most diverse scientific user facilities in the world. The NSLS, commissioned in 1982, has consistently operated at >95% reliability 24 hours a day, 7 days a week, with scheduled periods for maintenance and machine studies. Adding to its breadth is the fact that the NSLS consists of two distinct electron storage rings. The x-ray storage ring is 170 meters in circumference and can accommodate 60 beamlines or experimental stations, and the vacuum-ultraviolet (VUV) storage ring can provide 25 additional beamlines around its circumference of 51 meters. Synchrotron light from the x-ray ring is used to determine the atomic structure of materials using diffraction, absorption, and imaging techniques. Experiments at the VUV ring help solve the atomic and electronic structure as well as the magnetic properties of a wide array of materials. These data are fundamentally important to virtually all of the physical and life sciences as well as providing immensely useful information for practical applications. The petroleum industry, for example, uses the NSLS to develop new catalysts for refining crude oil and making by-products like plastics.

### Advanced Scientific Computing Research

BNL conducts basic research in applied mathematics and participates on SciDAC teams. It also participates in ISIC activities that focus on specific software challenges confronting users of terascale computers.

### Biological and Environmental Research

BNL operates beam lines for protein crystallography at the NSLS for use by the national biological research community, research in biological structure determination, and research into new instrumentation for detecting x-rays and neutrons. BNL conducts research into new instrumentation for detecting x-rays and neutrons. Research is also conducted on the molecular mechanisms of cell responses to low doses of radiation. BNL conducts molecular nuclear medicine research developing advanced medical imaging technologies including radiopharmaceuticals for medical imaging. The 2005 BER Distinguished Scientist for Medical Sciences is at BNL.

Climate change research includes the operation of the ARM External Data resource that provides ARM investigators with data from non-ARM sources, including satellite and ground-based systems. BNL scientists form an important part of the science team in the Atmospheric Sciences program (ASP), including providing special expertise in atmospheric field campaigns and aerosol research to the program. The ASP chief scientist is at BNL. BNL scientists play a leadership role in the operation of the Free-Air Carbon Dioxide Enrichment (FACE) facility at the Duke Forest used to understand how plants respond to elevated carbon dioxide concentrations in the atmosphere.

BNL supports environmental remediation sciences research and is participating in the National Science Foundation (NSF)/DOE Environmental Molecular Sciences Institute at State University of New York-Stony Brook and has instituted a new internal initiative EnviroSuite to support a growing community of environmental users at NSLS.

### High Energy Physics

The HEP program supports physics research and technology R&D at BNL, using unique resources of the laboratory, including engineering and technology for future accelerators and detectors, computational resources, and the Accelerator Test Facility.

**Nuclear Physics**

Research activities include use of relativistic heavy-ion beams and polarized protons in the Relativistic Heavy Ion Collider (RHIC) to investigate hot, dense nuclear matter and to understand the internal "spin" structure of the proton, respectively—parts of which are coordinated with the RIKEN BNL Research Center funded by Japan; development of future detectors for RHIC; a smaller R&D activity directed towards the ATLAS detector within the heavy-ion program at the LHC at CERN; research on the properties of neutrinos at the Sudbury Neutrino Observatory (SNO); a theory program emphasizing RHIC heavy ion and "spin" physics; and data compilation and evaluation at the National Nuclear Data Center (NNDC) that is the central U.S. site for these national and international efforts.

The **Relativistic Heavy Ion Collider** Facility, completed in 1999, is a major unique international facility currently used by about 1,000 scientists from 19 countries. RHIC uses Tandem Van de Graaff, Booster Synchrotron, and Alternating Gradient Synchrotron (AGS) accelerators in combination to inject beams into two rings of superconducting magnets of almost 4 kilometers circumference with 6 intersection regions where the beams can collide. It can accelerate and collide a variety of heavy ions, including gold beams, up to an energy of 100 GeV per nucleon. RHIC is being used to search for the predicted "quark-gluon plasma," a form of nuclear matter thought to have existed microseconds after the "Big Bang." It can also collide polarized protons with beams of energy up to 250 GeV per nucleon: a unique capability. Four detectors have been fabricated to provide complementary measurements, with some overlap in order to cross-calibrate the measurements. (1) The core of the Solenoidal Tracker at RHIC (STAR) detector is a large Time Projection Chamber (TPC) located inside a solenoidal magnet that tracks thousands of charged particles emanating from a single head-on gold-gold collision. A large modular barrel Electro-Magnetic Calorimeter (EMCal) and end-cap calorimeter measure deposited energy for high-energy charged and neutral particles and contain particle-photon discrimination capability. Other ancillary detector systems include a Silicon Vertex Tracker and forward particle tracking capabilities. A barrel Time of Flight detector upgrade (STAR TOF) is being added to significantly extend the particle identification capability of STAR detector. (2) The Pioneering High-Energy Nuclear Interacting eXperiment (PHENIX) detector has a particular focus on the measurement of rare probes at high event detection rate. It consists of two transverse spectrometer arms that can track charged particles within a magnetic field, especially to higher momentum: it provides excellent discrimination among photons, electrons, and hadrons. There are also two large muon tracking and identification systems in the forward and backward directions as well as ancillary tracker systems. Scientists using the other two smaller detectors, Phobos and Broad RAnge Hadron Magnetic Spectrometer (BRAHMS), have or are expected to complete their research programs and focus on data analysis in the near future. International participation has been essential in the implementation of all four detector systems.

The **Alternating Gradient Synchrotron** provides high intensity pulsed proton beams up to 33 GeV on fixed targets and secondary beams of kaons, muons, pions, and anti-protons. The AGS is the injector of (polarized) proton and heavy-ion beams into RHIC, and its operations are supported by the Heavy Ion subprogram as part of the RHIC facility. The AGS is also utilized for radiation damage studies of electronic systems for NASA supported work, among a variety of uses, with the support for these activities being provided by the relevant agencies.

The **Booster Synchrotron**, part of the RHIC injector, is providing heavy-ion beams to a dedicated beam line (NASA Space Radiation Laboratory) for biological and electronic systems radiation studies funded by NASA. The incremental costs for these studies are provided by NASA.

The **Tandem Van de Graaff** accelerators which serve as injectors for the Booster Synchrotron will be replaced by a modern, compact Electron Beam Ion Source (EBIS) and linac system which promises greater efficiency, greater reliability, and lower maintenance costs as well as the potential for future upgrades. The EBIS is a joint DOE/NASA project.

The **National Nuclear Data Center (NNDC)** is the central U.S. site for national and international nuclear data and compilation efforts. The U.S. Nuclear Data program is the United States' repository for information generated in low- and intermediate-energy nuclear physics research worldwide. This information consists of both bibliographic and numeric data. The NNDC is a resource for a very broad user community in all aspects of nuclear technology, with relevance to homeland security. Nuclear Data program-funded scientists at U.S. national laboratories and universities contribute to the activities and responsibilities of the NNDC.

**Science Laboratories Infrastructure**

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

**Safeguards and Security**

The Safeguards and Security (S&S) program activities are focused on protective forces, cyber security, personnel security, security systems, information security, program management, and material control and accountability. BNL operates a transportation division to move special nuclear materials around the site. Material control and accountability efforts focus on accurately accounting for and protecting the site's special nuclear materials.

## Brookhaven Site Office

### Introduction

The Brookhaven Site Office provides the single federal presence with responsibility for contract performance at the Brookhaven National Laboratory (BNL). This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Chicago Office

### Introduction

The Chicago Office supports the Department's programmatic missions in Science and Technology, National Nuclear Security, Energy Resources, and Environmental Quality by providing expertise and assistance in such areas as contract management, procurement, project management, engineering, facilities and infrastructure, property management, construction, human resources, financial management, general and patent law, environmental protection, quality assurance, integrated safety management, integrated safeguards and security management, nuclear material control and accountability, and emergency management. Chicago directly supports site offices responsible for program management oversight of seven major management and operating laboratories—Ames Laboratory, Argonne National Laboratory, Lawrence Berkeley National Laboratory, Brookhaven National Laboratory, Fermi National Accelerator Laboratory, Princeton Plasma Physics Laboratory, and Stanford Linear Accelerator Center—and one government-owned and government-operated Federal laboratory, New Brunswick Laboratory. Additionally, the administrative, business and technical expertise of Chicago is shared SC-wide through the Integrated Support Center concept. Chicago serves as SC's grant center, administering grants to 272 colleges/universities in all 50 states, Washington, D.C., and Puerto Rico, as determined by the DOE-SC program offices as well as non-SC offices.

### Basic Energy Sciences

The BES program funds research at 190 academic institutions located in 48 states.

### Advanced Scientific Computing Research

The Advanced Scientific Computing Research (ASCR) program funds research at over 70 colleges/ universities located in 24 states supporting approximately 126 principal investigators.

### Biological and Environmental Research

The Biological and Environmental Research (BER) program funds research at some 220 institutions, including colleges/universities, private industry, and other federal and private research institutions located in 44 states.

### High Energy Physics

The HEP program supports about 260 research groups at more than 100 colleges and universities located in 36 states, Washington, D.C., and Puerto Rico. The strength and effectiveness of the university-based program is critically important to the success of the program as a whole.

### Nuclear Physics

The Nuclear Physics (NP) program funds 185 research grants at 90 colleges/universities located in 35 states and the District of Columbia. Among these are grants with the Triangle Universities Nuclear Laboratory (TUNL) which includes the High Intensity Gamma Source (HIGS) at the Duke Free Electron Laser Laboratory; Texas A&M (TAMU) Cyclotron; the Yale Tandem Van de Graaff; University of Washington Tandem Van de Graaff and Center for Experimental Nuclear and Particle Astrophysics (CENPA); and the newly established Research and Engineering Center at the Massachusetts Institute for Technology. These accelerator facilities offer niche capabilities and opportunities not available at the national user facilities, or many foreign low-energy laboratories, such as specialized sources and targets, opportunities for extended experiments, and specialized instrumentation. Also supported is the Institute for Nuclear Theory (INT) at the University of Washington, a premier international center for new initiatives and collaborations in nuclear theory research.

### Fusion Energy Sciences

The Fusion Energy Sciences (FES) program funds research at more than 50 colleges and universities located in approximately 30 states. FES also funds the DIII-D tokamak experiment and related programs at General Atomics, an industrial firm located in San Diego, California.

## Fermi National Accelerator Laboratory

### Introduction

Fermi National Accelerator Laboratory is a program-dedicated laboratory (High Energy Physics) located on a 6,800-acre site in Batavia, Illinois. The laboratory consists of 358 buildings (2.3 million gross square feet of space) with an average building age of 39 years. Fermilab is the largest U.S. laboratory for research in high-energy physics and is second only to CERN, the European Laboratory for Particle Physics. About 2,500 scientific users, scientists from universities and laboratories throughout the U.S. and around the world, use Fermilab for their research. Fermilab’s mission is the goal of high-energy physics: to understand matter at its deepest level, to identify its fundamental building blocks, and to understand how the laws of nature determine their interactions.

### Advanced Scientific Computing Research

Fermilab participates in some SciDAC teams.

### High Energy Physics

Fermilab operates the **Tevatron** accelerator and colliding beam facility, which consists of a four-mile ring of superconducting magnets and two large multi-purpose detectors, and is capable of accelerating protons and antiprotons to an energy of one trillion electron volts (1 TeV). The Tevatron is the highest energy proton accelerator in the world, and will remain so until the LHC begins commissioning at CERN in 2007. With the shutdown of the Large Electron-Positron (LEP) collider at CERN in 2000, the Tevatron became the only operating particle accelerator at the energy frontier. The Tevatron complex also includes the Booster and the Main Injector, pre-accelerators to the Tevatron. The Main Injector, which is used for the pre-acceleration of protons and production of antiprotons as a part of the Tevatron complex, is also used independently of the Tevatron for a 120 GeV fixed target program, including the **Neutrinos at the Main Injector (NuMI)** beamline which started operation in 2005. Fermilab is the principal experimental facility for HEP. The HEP program also supports physics research and technology R&D at Fermilab, using unique resources of the laboratory, including state-of-the-art engineering and technology for future generations of accelerators and detectors and computational resources.

### Science Laboratories Infrastructure

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

### Safeguards and Security

S&S program efforts are directed at maintaining protective force staffing and operations to protect personnel and the facility, and toward continuing the cyber security, program management, security systems, and material control and accountability programs to accurately account for and protect the facility's special nuclear materials. Limited funding increases would be applied to security systems and the Foreign Visits and Assignments program.

## Fermi Site Office

### Introduction

The Fermi Site Office provides the single federal presence with responsibility for contract performance at the Fermi National Accelerator Laboratory (Fermilab). This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Idaho National Laboratory

### Introduction

Idaho National Laboratory (INL) is a multiprogram laboratory located on 572,000 acres in Idaho Falls, Idaho. Within the laboratory complex are nine major applied engineering, interim storage, and research and development facilities.

**Basic Energy Sciences**

INL supports studies to understand and improve the life expectancy of material systems used in engineering.

**Biological and Environmental Research**

INL is conducting research in subsurface science relating to clean up of the nuclear weapons complex with an emphasis on subsurface science.

**Fusion Energy Sciences**

Since 1978, INL has been the lead laboratory for fusion safety. As such, it has helped to develop the fusion safety database that will demonstrate the environmental and safety characteristics of both nearer term fusion devices and future fusion power plants. Research at INL focuses on the safety aspects of magnetic fusion concepts for existing and future machines, such as a burning plasma experiment, and further developing our domestic safety database using existing collaborative arrangements to conduct work on international facilities. In addition, INL has expanded their research and facilities capabilities to include tritium science activities. INL has completed fabrication of the Safety and Tritium Applied Research (STAR) Facility, which is a small tritium laboratory where the fusion program can conduct tritium material science, chemistry, and safety experiments. The STAR Facility has been declared a National User Facility. INL also coordinates codes and standards within the ITER program.

## Lawrence Berkeley National Laboratory

**Introduction**

The Lawrence Berkeley National Laboratory is a multiprogram laboratory located in Berkeley, California, on a 200-acre site adjacent to the Berkeley campus of the University of California. The laboratory consists of 106 buildings (1.6 million gross square feet of space) with an average building age of 36 years. LBNL is dedicated to performing leading-edge research in the biological, physical, materials, chemical, energy, and computer sciences. The land is leased from the University of California.

**Basic Energy Sciences**

LBNL is home to major research efforts in materials and chemical sciences as well as to efforts in geosciences, engineering, and biosciences. Collocated with the University of California at Berkeley, the Laboratory benefits from regular collaborations and joint appointments with numerous outstanding faculty members. The Laboratory is the home to the research of many students and postdoctoral appointees. It is also the site of three Basic Energy Sciences (BES) supported user facilities—the Advanced Light Source (ALS), the Molecular Foundry, and the National Center for Electron Microscopy (NCEM).

The **Advanced Light Source** provides vacuum-ultraviolet light and x-rays for probing the electronic and magnetic structure of atoms, molecules, and solids, such as those for high-temperature superconductors. The high brightness and coherence of the ALS light are particularly suited for soft x-ray imaging of biological structures, environmental samples, polymers, magnetic nanostructures, and other inhomogeneous materials. Other uses of the ALS include holography, interferometry, and the study of molecules adsorbed on solid surfaces. The pulsed nature of the ALS light offers special opportunities for time resolved research, such as the dynamics of chemical reactions. Shorter wavelength x-rays are also used at structural biology experimental stations for x-ray crystallography and x-ray spectroscopy of proteins and other important biological macromolecules. The ALS is a growing facility with a lengthening portfolio of beamlines that has already been applied to make important discoveries in a wide variety of scientific disciplines. An ALS User Support Building (USB) will begin design in FY 2007.

The USB will provide high-quality user support space in sufficient quantity to accommodate the very rapid growth in the number of ALS users and to accommodate projected future expansion. The USB will contain staging areas for ALS experiments, space for a long beamline that will extend from the floor of the ALS into the USB, and temporary office space for visiting users.

The **National Center for Electron Microscopy** provides instrumentation for high-resolution, electron-optical microcharacterization of atomic structure and composition of metals, ceramics, semiconductors, superconductors, and magnetic materials. This facility contains one of the highest resolution electron microscopes in the U.S.

The Molecular Foundry provides users with instruments, techniques, and collaborators to enhance the study of the synthesis, characterization, and theory of nanoscale materials. Its focus is on the multidisciplinary development and understanding of both “soft” (biological and polymer) and “hard” (inorganic and microfabricated) nanostructured building blocks and the integration of these building blocks into complex functional assemblies. Scientific themes include inorganic nanostructures; nanofabrication; organic, polymer, and biopolymer nanostructures; biological nanostructures; imaging and manipulation of nanostructures; and theory of nanostructures. The facility offers expertise in a variety of techniques for the study of nanostructures, including electronic structure and excited-state methods, *ab initio* and classical molecular dynamics, quantum transport, and classical and quantum Monte Carlo approaches. Several research laboratories at LBNL with capabilities that complement those at the facilities also are open to Foundry users.

**Advanced Scientific Computing Research**

LBNL conducts basic research in the mathematics and computer science, as well as research in advanced computing software tools. It participates in several scientific application partnerships, including the partnership with the BES program in nanoscale science, and participates on a number of the SciDAC teams. LBNL manages the ESnet. ESnet is one of the worlds most effective and progressive science-related computer networks that provides worldwide access and communications to Department of Energy facilities. LBNL is also the site of the NERSC, which 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. LBNL participates in ISIC activities that focus on specific software challenges confronting users of terascale computers.

**Biological and Environmental Research**

LBNL is one of the major national laboratory partners forming the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing techniques and studies on the biological functions associated with the newly sequenced human DNA. The laboratory also conducts research on the molecular mechanisms of cell responses to low doses of radiation, on the use of model organisms to understand and characterize the human genome, and on microbial systems biology research as part of Genomics:GTL. The Chief Scientist for the Low Dose Radiation Research program and the 2005 BER Distinguished Scientists for Environmental Remediation and for Life Sciences are at LBNL. LBNL operates beam lines for determination of protein structure at the ALS for use by the national and international biological research community. The ALS is also used by a growing environmental science community. LBNL also supports the environmental remediation sciences research and the geophysical and biophysical and biochemical research capabilities for field sites in that program.

LBNL conducts research on carbon cycling and carbon sequestration on terrestrial ecosystems. It also conducts research on biological and ecological responses to climatic and atmospheric changes.

LBNL conducts research into new technologies for the detailed characterization of complex environmental contamination. It also develops scalable implementation technologies that allow widely used climate models to run effectively and efficiently on massively parallel processing supercomputers. LBNL also conducts research on terrestrial carbon cycling to understand the processes controlling the exchange of $CO_2$ between terrestrial ecosystems and the atmosphere.

**High Energy Physics**

The HEP program supports physics research and technology R&D at LBNL, using unique capabilities of the laboratory in the areas of superconducting magnet R&D, engineering and detector technology, world-forefront expertise in laser driven particle acceleration, expertise in design of advanced electronic devices, computational resources, and design of modern, complex software codes for HEP experiments.

**Nuclear Physics**

The Low Energy subprogram has supported operations and the research program of the 88-Inch Cyclotron, whose operations transitioned in FY 2004 from a national user facility to a dedicated in-house facility with partial operational support from other federal agencies to carry out their programs. Other activities include fabrication of a next-generation gamma-ray detector system, GRETINA; research with the STAR detector located at Brookhaven's RHIC facility; development of future detector systems for RHIC; operation of the Parallel Distributed Systems Facility aimed at heavy-ion and low energy physics computation; R&D and conceptual design activities directed towards a detector upgrade for the ALICE detector heavy-ion program at the Large Hadron Collider (LHC) at Organisation Europέanne pour la Recherche Nucléaire (CERN); operation of the Sudbury Neutrino Observatory (SNO) detector in Canada and the KamLAND detector in Japan that are performing neutrino studies; development of next generation neutrino detectors; a theory program with an emphasis on relativistic heavy-ion physics; data compilation and evaluation activities supporting the National Nuclear Data Center at BNL; and a technical effort in generic R&D of rare isotope beam development with the development of electron-cyclotron resonance (ECR) ion sources.

**Fusion Energy Sciences**

LBNL has been conducting research in developing ion beams for applications to high energy density physics in the near term (4 to 10 years) and inertial fusion energy in the long term. Currently the laboratory has two major experimental systems for doing this research: the Neutralized Drift Compression Experiment (NDCX) and the High Current Experiment (HCX). Both experiments are directed at answering the question of how ion beams can be produced with the intensity required for research in high energy density physics and inertial fusion. LBNL conducts this research together with the Lawrence Livermore National Laboratory and Princeton Plasma Physics Laboratory through the Heavy Ion Fusion Virtual National Laboratory.

**Science Laboratories Infrastructure**

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

**Safeguards and Security**

This program provides physical protection of personnel and laboratory facilities. This is accomplished with protective forces, security systems, cyber security, program management, personnel security, and material control and accountability of special nuclear material.

## Lawrence Livermore National Laboratory

### Introduction

Lawrence Livermore National Laboratory (LLNL) is a multiprogram laboratory located on 821 acres in Livermore, California. This laboratory was built in Livermore as a weapons laboratory 42 miles from the campus of the University of California at Berkeley to take advantage of the expertise of the university in the physical sciences.

### Basic Energy Sciences

LLNL supports research in materials sciences and in geosciences research on the sources of electromagnetic responses in crustal rocks, seismology theory and modeling, the mechanisms and kinetics of low-temperature geochemical processes and the relationships among reactive fluid flow, geochemical transport, and fracture permeability.

### Advanced Scientific Computing Research

LLNL participates in base applied mathematics and computer science research and SciDAC efforts. It also participates in ISIC activities that focus on specific software challenges confronting users of terascale computers.

### Biological and Environmental Research

LLNL is one of the major national laboratory partners that comprise the Joint Genome Institute (JGI) whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. LLNL is developing new biocompatible materials and microelectronics for the artificial retina project. It also conducts research on the molecular mechanisms of cell responses to low doses of radiation, and on the use of model organisms to understand and characterize the human genome.

Through the program for Climate Model Diagnosis and Intercomparison, LLNL provides the international leadership to develop and apply diagnostic tools to evaluate the performance of climate models and to improve them. Virtually every climate modeling center in the world participates in this unique program. It also conducts research to improve understanding of the climate system, particularly the climate effect of clouds and aerosol properties and processes and climate change feedbacks on carbon cycling. The 2005 BER Distinguished Scientist for Climate Change Research is at LLNL.

### High Energy Physics

The HEP program supports physics research and technology R&D at LLNL, using unique capabilities of the laboratory primarily in the areas of engineering and detector technology and advanced accelerator R&D.

### Nuclear Physics

The LLNL program supports research in relativistic heavy-ion physics as part of the PHENIX collaboration at RHIC and the ALICE experiment at the CERN LHC, in nuclear data and compilation activities, on theoretical nuclear structure studies, and a technical effort involved in generic R&D of rare isotope beam development.

### Fusion Energy Sciences

LLNL works with LBNL and PPPL through the Heavy-Ion Fusion Virtual National Laboratory in advancing the physics of heavy ion beams as a driver for inertial fusion energy in the long term and high energy density physics in the near term. It also conducts research in the concept of Fast Ignition for applications in high energy density physics and inertial fusion energy. The LLNL program also includes collaborations with General Atomics on the DIII-D tokamak, operation of an innovative concept experiment, the Sustained Spheromak Physics Experiment at LLNL, and benchmarking of fusion physics computer models with experiments such as DIII-D. It carries out research in the simulation of turbulence and its effect on transport of heat and particles in magnetically confined plasmas. In addition, LLNL carries out research in support of magnets and plasma chamber and plasma-material interactions.

**Science Laboratories Infrastructure**

The SLI program enables the cleanup and removal of excess SC facilities at LLNL.

**Los Alamos National Laboratory**

**Introduction**

Los Alamos National Laboratory (LANL) is a multiprogram laboratory located on 27,000 acres in Los Alamos, New Mexico.

**Basic Energy Sciences**

LANL is home to a few efforts in materials sciences, chemical sciences, geosciences, and engineering. LANL supports research on strongly correlated electronic materials, high-magnetic fields, microstructures, deformation, alloys, bulk ferromagnetic glasses, mechanical properties, ion enhanced synthesis of materials, metastable phases and microstructures, and mixtures of particles in liquids.

Research is also supported to understand the electronic structure and reactivity of actinides through the study of organometallic compounds. Also supported is work to understand the chemistry of plutonium and other light actinides in both near-neutral pH conditions and under strongly alkaline conditions relevant to radioactive wastes and research in physical electrochemistry fundamental to energy storage systems. In the areas of geosciences, experimental and theoretical research is supported on rock physics, seismic imaging, the physics of the earth's magnetic field, fundamental geochemical studies of isotopic equilibrium/disequilibrium, and mineral-fluid-microbial interactions.

LANL is also the site of two BES supported user facilities: the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) and the Center for Integrated Nanotechnologies (CINT).

The **Manuel Lujan Jr. Neutron Scattering Center** provides an intense pulsed source of neutrons to a variety of spectrometers for neutron scattering studies. The Lujan Center features instruments for measurement of high-pressure and high-temperature samples, strain measurement, liquid studies, and texture measurement. The facility has a long history and extensive experience in handling actinide samples. A 30 Tesla magnet is also available for use with neutron scattering to study samples in high-magnetic fields. The Lujan Center is part of the Los Alamos Neutron Science Center (LANSCE), which is comprised of a high-power 800-MeV proton linear accelerator, a proton storage ring, production targets to the Lujan Center and the Weapons Neutron Research facility, and a variety of associated experiment areas and spectrometers for national security research and civilian research.

The **Center for Integrated Nanotechnologies** provides tools and expertise to explore the continuum from scientific discovery to the integration of nanostructures into the microworld and the macroworld. CINT is devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials. Through its core facility in Albuquerque, New Mexico, and its gateways to both Sandia National Laboratories and Los Alamos National Laboratory, CINT will provide access to tools and expertise to explore the continuum from scientific discovery to the integration of nanostructures into the microworld and the macroworld. CINT supports five scientific thrusts that serve as synergistic building blocks for integration research: nano-bio-micro interfaces, nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and theory and simulation.

**Advanced Scientific Computing Research**

LANL conducts basic research in the mathematics and computer science and in advanced computing software tools. It also participates in several scientific application partnerships and participates on a number of the SciDAC teams. LANL participates in ISIC activities that focus on specific software challenges confronting users of terascale computers.

**Biological and Environmental Research**

LANL is one of the major national laboratory partners that comprise the JGI whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. One of LANL's roles in the JGI involves the production of high quality "finished" DNA sequence. It also conducts research on the molecular mechanisms of cell responses to low doses of radiation and on research to understand the molecular control of genes and gene pathways in microbes. Activities in structural biology include the operation of an experimental station for protein crystallography at the LANSCE for use by the national biological research community.

LANL provides the site manager for the Tropical Western Pacific ARM site. LANL also has a crucial role in the development, optimization, and validation of coupled atmospheric and oceanic general circulation models using massively parallel computers. LANL also conducts research into advanced medical imaging technologies for studying brain function including optical imaging and magnetoencephology, novel radionuclide dosimetry and therapy, and research into new techniques for rapid characterization and sorting of mixtures of cells and cell fragments. LANL also conducts research under environmental remediation sciences with an emphasis on biological processes associated with plutonium mobility in the environment. LANL is participating in the National Science Foundation (NSF)/DOE Environmental Molecular Sciences Institute at the Pennsylvania State University.

**High Energy Physics**

The HEP program supports physics research and technology R&D at LANL, using unique capabilities of the laboratory primarily in the areas of theoretical studies, engineering, and detector technology.

**Nuclear Physics**

NP supports a broad program of research including: a program of neutron beam research that utilized beams from LANSCE facility to make fundamental physics measurements (to be completed in FY 2006); the conceptual design and R&D of an experiment to search for the electric dipole moment of the neutron; a research and development effort in relativistic heavy-ions using the PHENIX detector at the RHIC and development of next generation instrumentation for RHIC; research directed at the study of the quark substructure of the nucleon in experiments at Fermilab, and the "spin" structure of nucleons at RHIC using polarized proton beams; research at the Sudbury Neutrino Observatory (SNO) and at MiniBooNE directed at studies of the properties of neutrinos including development of the next generation detector; a broad program of theoretical research; nuclear data and compilation activities as part of the U.S. Nuclear Data program; and a technical effort involved in rare isotope beam development.

**Fusion Energy Sciences**

LANL has developed a substantial experimental system for research in Magnetized Target Fusion, one of the major innovative confinement concepts in magnetic alternates. The laboratory leads research in a high-density, compact plasma configuration called Field Reversed Configuration. LANL supports the creation of computer codes for modeling the stability of magnetically confined plasmas, including tokamaks and innovative confinement concepts. The work also provides theoretical and computational support for the Madison Symmetric Torus experiment, a proof-of-principle experiment in reversed field pinch at the University of Wisconsin in Madison. LANL develops advanced diagnostics for the National Spherical Torus Experiment (NSTX) at PPPL and other fusion experiments, such as the Rotating Magnetic Field as a current drive mechanism for the Field Reversed Configuration Experiment at the University of Washington in Seattle. The laboratory is also doing research in Inertial Electrostatic Confinement, another innovative confinement concept. LANL also supports the tritium processing activities needed for ITER.

## National Renewable Energy Laboratory

### Introduction

The National Renewable Energy Laboratory (NREL) is a program-dedicated laboratory (Solar) located on 300 acres in Golden, Colorado. NREL was built to emphasize renewable energy technologies such as photovoltaics and other means of exploiting solar energy. It is the world leader in renewable energy technology development. Since its inception in 1977, NREL's sole mission has been to develop renewable energy and energy efficiency technologies and transfer these technologies to the private sector.

### Basic Energy Sciences

NREL supports basic research efforts that underpin this technological emphasis at the laboratory; e.g., on overcoming semiconductor doping limits, novel and ordered semiconductor alloys, and theoretical and experimental studies of properties of advanced semiconductor alloys for prototype solar cells. It also supports research addressing the fundamental understanding of solid-state, artificial photosynthetic systems. This research includes the preparation and study of novel dye-sensitized semiconductor electrodes, characterization of the photophysical and chemical properties of quantum dots, and study of charge carrier dynamics in semiconductors.

## Oak Ridge Institute for Science and Education

### Introduction

The Oak Ridge Institute for Science and Education, operated by Oak Ridge Associated Universities (ORAU), is located on a 150-acre site in Oak Ridge, Tennessee. Established in 1946, ORAU is a university consortium leveraging the scientific strength of major research institutions to advance science and education by partnering with national laboratories, government agencies, and private industry. ORISE focuses on scientific initiatives to research health risks from occupational hazards, assess environmental cleanup, respond to radiation medical emergencies, support national security and emergency preparedness, and educate the next generation of scientists.

### Basic Energy Sciences

ORISE supports a consortium of university and industry scientists to share the ORNL research station at NSLS to study the atomic and molecular structure of matter (known as ORSOAR, the Oak Ridge Synchrotron Organization for Advanced Research). ORISE provides administrative support for panel reviews and site reviews. It also assists with the administration of topical scientific workshops and provides administrative support for other activities such as for the reviews of construction projects. ORISE manages the **Shared Research Equipment (SHaRE)** program at ORNL. The SHaRE program makes available state-of-the-art electron beam microcharacterization facilities for collaboration with researchers from universities, industry, and other government laboratories.

### Advanced Scientific Computing Research

ORISE provides support for education activities.

### Biological and Environmental Research

ORISE coordinates research fellowship programs and manages the DOE-NSF program supporting graduate students to attend the Lindau Meeting of Nobel Laureates. It also coordinates activities associated with the peer review of most of the submitted research proposals.

### High Energy Physics

ORISE provides support to the HEP program in the area of program planning and review.

### Nuclear Physics

ORISE supports the Holifield Radioactive Ion Beam Facility (HRIBF) and its research program through a close collaboration with university researchers using HRIBF.

### Fusion Energy Sciences

ORISE supports the operation of the Fusion Energy Sciences Advisory Committee (FESAC) and administrative aspects of some FES program peer reviews. It also acts as an independent and unbiased agent to administer the FES Graduate and Postgraduate Fellowship programs, in conjunction with FES, the ORO, participating universities, DOE laboratories, and industries.

### Science Laboratories Infrastructure

The SLI program enables the cleanup and removal of excess facilities at the facility.

### Safeguards and Security

The S&S program at ORISE provides physical protection/protective force services by employing unarmed security officers. The facilities are designated as property protection areas for the purpose of protecting government-owned assets. In addition to the government-owned facilities and personal property, ORISE possesses small quantities of nuclear materials that must be protected. The program includes information security, program management, personnel security, protective forces, security systems, and cyber security.

## Oak Ridge National Laboratory

### Introduction

The Oak Ridge National Laboratory is a multiprogram laboratory located on the 24,000 acre reservation at Oak Ridge, Tennessee. The laboratory's 1,100 acre main site on Bethel Valley Road contains 303 buildings (3.5 million gross square feet of space) with an average building age of 35 years. Scientists and engineers at ORNL conduct basic and applied research and development to create scientific knowledge and technological solutions that strengthen the nation's leadership in key areas of science; increase the availability of clean, abundant energy; restore and protect the environment; and contribute to national security. The laboratory supports almost every major Departmental mission in science, defense, energy resources, and environmental quality. It provides world-class scientific research capability while advancing scientific knowledge through such major Departmental initiatives as the Spallation Neutron Source (SNS), the Supercomputing Program, Nanoscience Research, complex biological systems, and ITER. In the defense mission arena, programs include those which protect our Homeland and National Security by applying advanced science and nuclear technology to the Nation's defense. Through the Nuclear Nonproliferation Program, Oak Ridge supports the development and coordination of the implementation of domestic and international policy aimed at reducing threats, both internal and external, to the U.S. from weapons of mass destruction. The Laboratory also supports various Energy Efficiency and Renewable Energy programs and facilitates the R&D of energy efficiency and renewable energy technologies.

**Basic Energy Sciences**

ORNL is home to major research efforts in materials and chemical sciences with additional programs in engineering and geosciences. ORNL has perhaps the most comprehensive materials research program in the country. It is also the site of three BES supported user facilities—the Spallation Neutron Source (SNS), which is under construction and scheduled for commissioning in FY 2006; the High Flux Isotope Reactor (HFIR); and the Center for Nanophase Materials Sciences (CNMS). ORNL has perhaps the most comprehensive materials research program in the country.

The **Spallation Neutron Source** is a next-generation short-pulse spallation neutron source for neutron scattering that is significantly more powerful (by about a factor of 10) than the best spallation neutron source now in existence. The SNS consists of a linac-ring accelerator system that delivers short (microsecond) proton pulses to a target/moderator system where neutrons are produced by a process called spallation. The neutrons so produced are then used for neutron scattering experiments. Specially designed scientific instruments use these pulsed neutron beams for a wide variety of investigations. There is initially one target station that can accommodate 24 instruments; the potential exists for adding more instruments and a second target station later.

The **High Flux Isotope Reactor** is a light-water cooled and moderated reactor that began full-power operations in 1966. HFIR operates at 85 megawatts to provide state-of-the-art facilities for neutron scattering, materials irradiation, and neutron activation analysis and is the world's leading source of elements heavier than plutonium for research, medicine, and industrial applications. The neutron scattering experiments at HFIR reveal the structure and dynamics of a very wide range of materials. The neutron-scattering instruments installed on the four horizontal beam tubes are used in fundamental studies of materials of interest to solid-state physicists, chemists, biologists, polymer scientists, metallurgists, and colloid scientists. Recently, a number of improvements at HFIR have increased its neutron scattering capabilities to 14 state-of-the-art neutron scattering instruments on the world's brightest beams of steady-state neutrons. These upgrades include the installation of larger beam tubes and shutters, a high-performance liquid hydrogen cold source, and neutron scattering instrumentation.

The **Center for Nanophase Materials Sciences** integrates nanoscale science with neutron science; synthesis science; and theory, modeling, and simulation. Scientific themes include macromolecular complex systems, functional nanomaterials such as carbon nanotubes, nanoscale magnetism and transport, catalysis and nano building blocks, and nanofabrication.

**Advanced Scientific Computing Research**

ORNL conducts basic research in the mathematics and computer science, as well as research in advanced computing software tools. It also participates in several scientific application partnerships and participates on a number of the SciDAC teams. Integrated Software Infrastructure Center activities are focused on specific software challenges confronting users of terascale computers. The Center for Computational Sciences (CCS), located at ORNL, provides high-end capability computing services to SciDAC teams and other DOE users. ORNL was selected by DOE to develop Leadership Computing Facility (LCF) for science to revitalize the U.S. effort in high end computing.

### Biological and Environmental Research

ORNL has a leadership role in research focused on the ecological aspects of global environmental change. It supports basic research through ecosystem-scale manipulative experiments in the field, through laboratory experiments involving model ecosystems exposed to global change factors, and through development and testing of computer simulation models designed to explain and predict effects of climatic change on the structure and functioning of terrestrial ecosystems. ORNL is the home of a FACE experiment which facilitates research on terrestrial carbon processes and the development of terrestrial carbon cycle models. It also houses the ARM archive, providing data to ARM scientists and to the general scientific community. ORNL, in conjunction with ANL and PNNL and six universities, plays a principle role in the CSiTE consortium which is focusing on research to enhance the capacity, rates, and longevity of carbon sequestration in terrestrial ecosystems. ORNL scientists provide improvement in formulations and numerical methods necessary to improve climate models. ORNL scientists make important contributions to the environmental remediation sciences research programs, providing special leadership in microbiology applied in the field. ORNL also manages the environmental remediation sciences research Field Research Center, a field site for developing and testing bioremediation methods for metal and radionuclide contaminants in subsurface environments.

ORNL is one of the major national laboratory partners that comprise the JGI whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. One of ORNL's roles in the JGI involves the annotation (assigning biological functions to genes) of completed genomic sequences and mouse genetics. ORNL conducts research on widely used data analysis tools and information resources that can be automated to provide information on the biological function of newly discovered genes identified in high-throughput DNA sequencing projects. ORNL conducts microbial systems biology research as part of Genomics:GTL. The laboratory also operates the Laboratory for Comparative and Functional Genomics, or "Mouse House," which uses mice as model organisms to understand and characterize the human genome. The laboratory conducts research into new instrumentation for the analytical chemistry of complex environmental contamination using new types of biosensors. The laboratory is developing a new experimental station for biological small angle neutron scattering.

### High Energy Physics

The HEP program supports a small research effort using unique capabilities of ORNL primarily in the area of particle beam shielding calculations.

### Nuclear Physics

The major effort at ORNL is the research, development, and operations of the HRIBF that is operated as a National User Facility. Also supported are a relativistic heavy-ion group that is involved in a research program using the PHENIX detector at RHIC and ALICE at the LHC; the development of the Fundamental Neutron Physics Beamline at SNS; a theoretical nuclear physics effort that emphasizes investigations of nuclear structure and astrophysics; nuclear data and compilation activities that support the national nuclear data effort; and a technical effort involved in rare isotope beam development.

The **Holifield Radioactive Ion Beam Facility** is the only radioactive nuclear beam facility in the U.S. to use the isotope separator on-line (ISOL) method and is used annually by about 90 scientists for studies in nuclear structure, dynamics, and astrophysics using radioactive beams. The HRIBF accelerates secondary radioactive beams to higher energies (up to 10 MeV per nucleon) than any other facility in the world with a broad selection of ions. The HRIBF conducts R&D on ion sources and low energy ion transport for radioactive beams. The capabilities of HRIBF are being augmented by the construction of the High Power Test Laboratory (HPTL) which will provide capabilities which will be unique in the world for the development and testing of new ion source techniques.

**Fusion Energy Sciences**

ORNL develops a broad range of components that are critical for improving the research capability of fusion experiments located at other institutions and that are essential for developing fusion as an environmentally acceptable energy source. The laboratory is a leader in the theory of heating of plasmas by electromagnetic waves, antenna design, and design and modeling of pellet injectors to fuel the plasma and control the density of plasma particles. The laboratory is also the site of the Controlled Fusion Atomic Data Center and its supporting research programs. While some ORNL scientists are located full-time at off-site locations, others carry out their collaborations with short visits to the host institutions, followed by extensive computer communications from ORNL for data analysis and interpretation, and theoretical studies. ORNL is also a leader in stellarator theory and design and is a major partner with PPPL on the National Compact Stellarator Experiment (NCSX) being built at PPPL. ORNL, in partnership with PPPL, shares responsibility for managing the U.S. ITER Project Office, effective July 2004. ORNL has led the fusion materials science program. This program will be reduced significantly in FY 2007.

**Science Laboratories Infrastructure**

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

**Safeguards and Security**

The S&S program includes security systems, information security, cyber security, personnel security, material control and accountability, and program management. Program planning functions at the laboratory provide for short- and long-range strategic planning, and special safeguards plans associated with both day-to-day protection of site-wide security interests and preparation for contingency operations. Additionally, ORNL is responsible for providing overall laboratory policy direction and oversight in the security arena; for conducting recurring programmatic self-assessments; for assuring a viable ORNL Foreign Ownership, Control or Influence (FOCI) program is in place; and for identifying, tracking, and obtaining closure on findings or deficiencies noted during inspections, surveys, or assessments of S&S programs.

## Oak Ridge Office

### Introduction

The Oak Ridge Office (ORO) directly provides corporate support (i.e., procurement, legal, finance, budget, human resources, and facilities and infrastructure) to site offices responsible for program management oversight of two major management and operating laboratories: PNNL and TJNAF. Oak Ridge also oversees the Oak Ridge Reservation and other DOE facilities in the City of Oak Ridge. Together on the Reservation and in the City of Oak Ridge there are 24 buildings (362,700 square feet) with a total replacement plant value (RPV) of $29.0 million. The RPV of the roads and other structures on the Reservation is $48.2 million. As a result of the recent A-76 competition for financial services, the Oak Ridge Financial Service Center provides payment services for the entire Department of Energy/NNSA, nation-wide. The administrative, business, and technical expertise of Oak Ridge is shared SC-wide through the Integrated Support Center concept. The ORO Manager is also the single Federal official with responsibility for contract performance at ORNL and the Oak Ridge Institute for

Science and Education (ORISE). The Manager provides on-site presence for ORNL and ORISE with authority encompassing contract management, program and project implementation, Federal stewardship, and internal operations.

**Science Laboratories Infrastructure**

The Oak Ridge Landlord subprogram provides for centralized ORO infrastructure requirements and general operating costs for activities (e.g., roads) on the Oak Ridge Reservation outside plant fences plus DOE facilities in the town of Oak Ridge, PILT, and other needs related to landlord activities.

**Safeguards and Security**

The S&S program provides for contractor protective forces for the Federal office building and ORNL. This includes protection of a category 1 Special Nuclear Material Facility, Building 3019. Other small activities include security systems, information security, and personnel security.

## Office of Scientific and Technical Information

**Introduction**

The Office of Scientific and Technical Information (OSTI) is located on an 8-acre site in Oak Ridge, Tennessee. The 134,000 square foot OSTI facility houses both Federal and contractor staff; the E-Government infrastructure handling over 15 million downloads and views of DOE's R&D results per year; and over 1.2 million classified and unclassified documents dating from the Manhattan Project to the present. These resources enable OSTI to fulfill its mission to advance science and sustain technological creativity by making R&D findings available and useful to DOE researchers and the American people. OSTI hosts web sites for BER programs and maintains on-line databases.

**Safeguards and Security**

The S&S program physical security is achieved through a graded protection system including protective forces, security systems, cyber security and program management. The S&S program also incorporates lock and key control, closed circuit television (CCTV), electronic access control and physical access control whereby visitors and employees attain building access via a lobby post where a receptionist is stationed.

## Pacific Northwest National Laboratory

**Introduction**

Pacific Northwest National Laboratory is a multiprogram laboratory located on 132 acres at the Department's Hanford site in Richland, Washington. The laboratory consists of one 8 year old government-owned building (200,000 gross square feet of space). PNNL conducts research in the area of environmental science and technology and carries out related national security, energy, and human health

**Basic Energy Sciences**

PNNL supports research in interfacial and surface chemistry, inorganic molecular clusters, analytical chemistry, and applications of theoretical chemistry to understanding surface. Geosciences research includes theoretical and experimental studies to improve our understanding of phase change phenomena in microchannels. Also supported is research on stress corrosion and corrosion fatigue, interfacial dynamics during heterogeneous deformation, irradiation assisted stress corrosion cracking, bulk defect and defect processing in ceramics, chemistry and physics of ceramic surfaces and interfacial deformation mechanisms in aluminum alloys.

### Advanced Scientific Computing Research

PNNL conducts basic research in the mathematics and computer science, as well as research in advanced computing software tools. It also participates in several scientific application partnerships, participates on a number of the SciDAC teams, and participates in Integrated Software Infrastructure Center activities that focus on specific software challenges confronting users of terascale computers.

### Biological and Environmental Research

PNNL is home to the William R. Wiley **Environmental Molecular Sciences Laboratory (EMSL),** a national scientific user facility. PNNL scientists, including EMSL scientists, play important roles in performing environmental remediation sciences research with representation in most areas within that program. PNNL operates the unique ultrahigh field mass spectrometry and nuclear magnetic resonance spectrometry instruments as well as a wide variety of other cutting edge analytical capabilities at the EMSL for use by the national research community.

PNNL provides expertise in research on aerosol properties and processes and in field campaigns for atmospheric sampling and analysis of aerosols. The Atmospheric Radiation Measurement (ARM) program office is located at PNNL, as is the project manager for the ARM engineering activity; this provides invaluable logistical, technical, and scientific expertise for the program. PNNL also conducts research on improving methods and models for assessing the costs and benefits of climate change and of various different options for mitigating and/or adapting to such charges. It also conducts research into new instrumentation for microscopic imaging of biological systems and for characterization of complex radioactive contaminants by highly automated instruments.

PNNL is one of the major national laboratory partners that comprise the JGI whose principal goals are high-throughput DNA sequencing and studies on the biological functions associated with newly sequenced human DNA. One of PNNL's roles in the JGI involves proteomics research (identifying all the proteins found in cells). PNNL conducts research on the molecular mechanisms of cell responses to low doses of radiation and on the development of high throughput approaches for characterizing all of the proteins (the proteome) being expressed by cells under specific environmental conditions. PNNL conducts microbial systems biology research as part of Genomics:GTL. The Chief Scientist for the Genomics: GTL program is at PNNL.

PNNL, in conjunction with ANL and ORNL and six universities, plays an important role in the CSiTE consortium, focusing on the role of soil microbial processes in carbon sequestration. PNNL also conducts research on the integrated assessment of global climate change.

### Fusion Energy Sciences

PNNL has focused on research on materials that can survive in a fusion neutron environment. Experienced scientists and engineers at PNNL provide leadership in the evaluation of ceramic matrix composites for fusion applications and support work on vanadium, copper, and ferrite steels as part of the U.S. fusion materials team. These programs will be reduced significantly in FY 2007.

### Science Laboratories Infrastructure

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

### Safeguards and Security

The PNNL S&S program consists of program management, physical security systems, protection operations, information security, cyber security, personnel security and material control and accountability.

## Pacific Northwest Site Office

### Introduction

The Pacific Northwest Site Office provides the single federal presence with responsibility for contract performance at PNNL. This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Princeton Plasma Physics Laboratory

### Introduction

Princeton Plasma Physics Laboratory (PPPL) is a program-dedicated laboratory (Fusion Energy Sciences) located on 88.5 acres in Plainsboro, New Jersey. The laboratory consists of 35 buildings (725,000 gross square feet of space) with an average building age of 30 years. DOE does not own the land.

### Advanced Scientific Computing Research

PPPL participates in several SciDAC projects.

### High Energy Physics

The HEP program supports a small theoretical research effort at PPPL using unique capabilities of the laboratory in the area of advanced accelerator R&D.

### Fusion Energy Sciences

PPPL is the only U.S. Department of Energy (DOE) laboratory devoted primarily to plasma and fusion science. The laboratory hosts experimental facilities used by multi-institutional research teams and also sends researchers and specialized equipment to other fusion facilities in the United States and abroad. PPPL is the host for the NSTX, which is an innovative toroidal confinement device, closely related to the tokamak, and has started construction of another innovative toroidal concept, the NCSX, a compact stellarator. PPPL scientists and engineers have significant involvement in the DIII-D and Alcator C-Mod tokamaks and the NSF Center for Magnetic Self-Organization in Laboratory and Astrophysical Plasmas in the U.S. and several large tokamak facilities abroad, including JET (Europe), JT-60U (Japan), and KSTAR (Korea). This research is focused on developing the scientific understanding and innovations required for an attractive fusion energy source. PPPL scientists are also involved in several basic plasma science experiments, ranging from magnetic reconnection to plasma processing. PPPL also has a large theory group that does research in the areas of turbulence and transport, equilibrium and stability, wave-plasma interaction, and heavy ion accelerator physics. PPPL, LBNL, and LLNL currently work together in advancing the physics of heavy ion drivers through the heavy ion beams Fusion Virtual National Laboratory. Effective July 2004, PPPL, in partnership with ORNL, was selected to manage the U.S. ITER Project Office. Through its association with Princeton University, PPPL provides high quality education in fusion-related sciences, having produced more than 185 Ph.D. graduates since its founding in 1951.

### Science Laboratories Infrastructure

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

### Safeguards and Security

The S&S program provides for protection of nuclear materials, government property, and other vital assets from unauthorized access, theft, diversion, sabotage, or other hostile acts. These activities result in reduced risk to national security and the health and safety of DOE and contractor employees, the public, and the environment. The PPPL S&S program consists of protective forces, security systems, cyber security, and program management.

## Princeton Site Office

### Introduction

The Princeton Site Office provides the single federal presence with responsibility for contract performance at the Princeton Plasma Physics Laboratory. This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Sandia National Laboratories

### Introduction

Sandia National Laboratories (SNL) is a multiprogram laboratory located on 3,700 acres in Albuquerque, New Mexico (SNL/NM), with sites in Livermore, California (SNL/CA), and Tonopah, Nevada.

### Basic Energy Sciences

SNL is home to significant research efforts in materials and chemical sciences with additional programs in engineering and geosciences. SNL/CA is also the site of the Combustion Research Facility (CRF). SNL has a historic emphasis on electronic components needed for Defense Programs. The laboratory has very modern facilities in which unusual microcircuits and structures can be fabricated out of various semiconductors. It is also the site of two BES supported user facilities—the Combustion Research Facility (CRF) and the Center for Integrated Nanotechnologies (CINT).

The **Combustion Research Facility** at SNL/CA is an internationally recognized facility for the study of combustion science and technology. In-house efforts combine theory, modeling, and experiment including diagnostic development, kinetics, and dynamics. Several innovative non-intrusive optical diagnostics such as degenerate four-wave mixing, cavity ring-down spectroscopies, high resolution optical spectroscopy, and ion-imaging techniques have been developed to characterize combustion intermediates. Basic research is often conducted in close collaboration with applied programs. A principal effort in turbulent combustion is coordinated among the chemical physics program, and programs in Fossil Energy and Energy Efficiency and Renewable Energy.

The **Center for Integrated Nanotechnologies** provides tools and expertise to explore the continuum from scientific discovery to the integration of nanostructures into the microworld and the macroworld. CINT is devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials. Through its core facility in Albuquerque, New Mexico, and its gateways to both Sandia National Laboratories and Los Alamos National Laboratory, CINT will provide access to tools and expertise to explore the continuum from scientific discovery to the integration of nanostructures into the microworld and the macroworld. CINT supports five scientific thrusts that serve as synergistic building blocks for integration research: nano-bio-micro interfaces, nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and theory and simulation.

**Advanced Scientific Computing Research**

SNL conducts basic research in mathematics and computer science, as well as research in advanced computing software tools. It also participates in several scientific application partnerships, participates on a number of the SciDAC teams, and participates in ISIC activities that focus on specific software challenges confronting users of terascale computers.

**Biological and Environmental Research**

SNL provides the site manager for the North Slope of Alaska ARM site. The chief scientist for the ARM-Unmanned Aerial Vehicles (UAV) program is at SNL, and SNL takes the lead role in coordinating and executing ARM-UAV missions. The laboratory conducts advanced research and technology development in robotics, smart medical instruments, microelectronic fabrication of the artificial retina, and computational modeling of biological systems, and fundamental chemistry for the treatment of high-level waste.

To support environmental cleanup, SNL conducts research into novel sensors for analytical chemistry of contaminated environments.

**Fusion Energy Sciences**

Sandia plays a lead role in developing components for fusion devices through the study of plasma interactions with materials, the behavior of materials exposed to high heat fluxes, and the interface of plasmas and the walls of fusion devices. It selects, specifies, and develops materials for components exposed to high heat and particles fluxes and conducts extensive analysis of prototypes to qualify components before their use in fusion devices. Materials samples and prototypes are tested in Sandia's Plasma Materials Test Facility, which uses high-power electron beams to simulate the high heat fluxes expected in fusion environments. Materials and components are exposed to tritium-containing plasmas in the Tritium Plasma Experiment located in the STAR facility at INL. Tested materials are characterized using Sandia's accelerator facilities for ion beam analysis. Sandia supports a wide variety of domestic and international experiments in the areas of tritium inventory removal, materials postmortem analysis, diagnostics development, and component design and testing. A number of these activities will be reduced in FY 2007. Sandia also works with LBNL through the Heavy Ion-Fusion Virtual National Laboratory in developing high-brightness ion source and other science issues of heavy ion beams. Sandia serves an important role in the design and analysis activities related to the ITER first wall components, including related R&D.

**Savannah River National Laboratory**

**Introduction**

The Savannah River National Laboratory (SRNL) is a multiprogram laboratory located on approximately 34 acres in Aiken, South Carolina. SRNL provides scientific and technical support for the site's missions, working in partnership with the site's operating divisions.

**Biological and Environmental Research**

SRNL scientists support environmental remediation sciences research program in the area of bioimmobilization of heavy metals and radionuclides.

## Stanford Linear Accelerator Center

### Introduction

The Stanford Linear Accelerator Center (SLAC) is located on 426 acres of Stanford University land in Menlo Park, California, and is also the home of the Stanford Synchrotron Radiation Laboratory (SSRL). The facility is now comprised of 25 experimental stations and is used each year by over 700 researchers from industry, government laboratories, and universities. SLAC (including SSRL) consists of 114 buildings (1.7 million gross square feet of space) with the average age of 29 years. SLAC is a laboratory dedicated to the design, construction, and operation of state-of-the-art electron accelerators and related experimental facilities for use in high-energy physics and synchrotron radiation research. SLAC operates the 2 mile long Stanford Linear Accelerator which began operating in 1966. The SSRL was built in 1974 to utilize the intense x-ray beams from the Stanford Positron Electron Accelerating Ring (SPEAR) that was built for particle physics by the SLAC laboratory. Over the years, SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third generation synchrotron sources.

### Basic Energy Sciences

SLAC is the home of the **Stanford Synchrotron Radiation Laboratory** and peer-reviewed research projects associated with SSRL. The facility is used by researchers from industry, government laboratories, and universities. These include astronomers, biologists, chemical engineers, chemists, electrical engineers, environmental scientists, geologists, materials scientists, and physicists. A research program is conducted at SSRL with emphasis in both the x-ray and ultraviolet regions of the spectrum. SSRL scientists are experts in photoemission studies of high-temperature superconductors and in x-ray scattering. The SPEAR 3 upgrade at SSRL provides major improvements that will increase the brightness of the ring for all experimental stations.

### Advanced Scientific Computing Research

SLAC participates on a number of SciDAC teams.

### Biological and Environmental Research

SLAC operates nine SSRL beam lines for structural molecular biology. This program involves synchrotron radiation-based research and technology developments in structural molecular biology that focus on protein crystallography, x-ray small angle scattering diffraction, and x-ray absorption spectroscopy for determining the structures of complex proteins of many biological consequences. Beamlines at SSRL also serve the growing environmental science user community.

### High Energy Physics

SLAC operates the **B-factory** and its detector, BaBar, and a small program of experiments in accelerator science and technology. The B-factory, a high energy electron-positron collider, was constructed to support a search for and high-precision study of CP symmetry violation in the B meson system. All of these facilities make use of the two-mile long linear accelerator, or linac. The HEP program also supports physics research and technology R&D at SLAC, using unique resources of the laboratory, including engineering and detector technology, advanced accelerator technology, and computational resources.

### Science Laboratories Infrastructure

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

#### Safeguards and Security

The S&S program focuses on reducing the risk to DOE national facilities and assets. The program consists primarily of protective forces, security systems, program management, and cyber security program elements.

### Stanford Site Office

#### Introduction

The Stanford Site Office provides the single federal presence with responsibility for contract performance at the Stanford Linear Accelerator Center (SLAC). This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

### Thomas Jefferson National Accelerator Facility

#### Introduction

Thomas Jefferson National Accelerator Facility is an Office of Science laboratory (Nuclear Physics) located on 162 acres (DOE-owned) in Newport News, Virginia focused on the exploration of nuclear and nucleon structure. The laboratory consists of 62 buildings with an average building age of 14 years, 2 state leased buildings, 23 real property trailers, and 10 other structures and facilities totaling over 764,000 gross square feet of space. The laboratory was constructed over the period FY 1987–1995.

#### Biological and Environmental Research

BER supports the development of advanced imaging instrumentation at TJNAF that will ultimately be used in the next generation medical imaging systems.

#### High Energy Physics

The HEP program supports an R&D effort at TJNAF on accelerator technology, using the unique expertise of the laboratory in the area of superconducting radiofrequency systems for particle acceleration.

#### Nuclear Physics

The centerpiece of TJNAF is the **Continuous Electron Beam Accelerator Facility (CEBAF)**, a unique international electron-beam user facility for the investigation of nuclear and nucleon structure based on the underlying quark substructure. The facility has a user community of ~1,200 researchers and is used annually by ~800 U.S. and foreign researchers. Polarized electron beams up to 5.7 GeV can be provided by CEBAF simultaneously to 3 different experimental halls. Hall A is designed for spectroscopy and few-body measurements. Hall B has a large acceptance detector, CLAS, for detecting multiple charged particles coming from a scattering reaction. Hall C is designed for flexibility to incorporate a wide variety of different experiments. Its core equipment consists of two medium resolution spectrometers for detecting high momentum or unstable particles. The G0 detector, a joint NSF-DOE project in Hall C, will allow a detailed mapping of the strange quark contribution to nucleon structure. Also in Hall C, a new detector, Q-weak, is being developed to measure the weak charge of the proton by a collaboration of laboratory and university groups in partnership with the NSF. TJNAF supports a group that does theoretical calculations and investigations in subjects supporting the experimental research programs in Medium Energy Physics. TJNAF research and engineering staff are world experts in Superconducting Radio-Frequency (SRF) accelerator technology; their expertise is being used in the development of the

12 GeV Upgrade for CEBAF as well as for other accelerator projects such as the Spallation Neutron Source.

**Science Laboratories Infrastructure**

The SLI program enables Departmental research missions at the laboratory by funding line item construction to maintain the general purpose infrastructure, and the cleanup and removal of excess facilities.

**Safeguards and Security**

TJNAF has a guard force (protective force) that provides 24-hour services for the accelerator site and after-hours property protection security for the entire site. Other security programs include cyber security, program management, material control and accountability, and security systems.

## Thomas Jefferson Site Office

### Introduction

The Thomas Jefferson Site Office provides the single federal presence with responsibility for contract performance at Thomas Jefferson National Accelerator Facility (TJNAF). This site office provides an on-site SC presence with authority encompassing contract management, program and project implementation, federal stewardship, and internal operations.

## Washington Headquarters

SC Headquarters, located in the Washington, D.C. area, supports the SC mission by funding Federal staff responsible for directing, administering, and supporting a broad spectrum of scientific disciplines. These disciplines include the HEP, NP, BES, BER, FES, ASCR, and WDTS programs. In addition, Federal staff are responsible for SC-wide management, operational policy, and technical/administrative support activities in budget and planning; information technology; infrastructure management; construction management; safeguards and security; environment, safety and health; and general administration. Funded expenses include salaries, benefits, travel, general administrative support services and technical expertise, information technology maintenance and enhancements, as well as other costs funded through interdepartmental transfers and interagency transfers.

# Basic Energy Sciences

## Funding Profile by Subprogram

(dollars in thousands)

| | FY 2005 Current Appropriation | FY 2006 Original Appropriation | FY 2006 Adjustments | FY 2006 Current Appropriation | FY 2007 Request |
|---|---|---|---|---|---|
| Basic Energy Sciences | | | | | |
| Research | | | | | |
| Materials Sciences and Engineering | 621,226 | 746,143 | -8,428[ab] | 737,715 | 1,004,212 |
| Chemical Sciences, Geosciences, and Energy Biosciences | 232,365 | 221,801 | -1,251[ab] | 220,550 | 268,499 |
| Total, Research | 853,591 | 967,944 | -9,679 | 958,265 | 1,272,711 |
| Construction | 230,025 | 178,073 | -1,781[a] | 176,292 | 148,269 |
| Total, Basic Energy Sciences | 1,083,616[c] | 1,146,017 | -11,460 | 1,134,557 | 1,420,980 |

**Public Law Authorizations:**
Public Law 95-91, "Department of Energy Organization Act, 1977"
Public Law 103-62, "Government Performance and Results Act of 1993"
Public Law 108-153, "21st Century Nanotechnology Research and Development Act of 2003"
Public Law 109-58, "Energy Policy Act of 2005"

## Mission

The mission of the BES program—a multipurpose, scientific research effort—is to foster and support fundamental research to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. The portfolio supports work in the natural sciences emphasizing fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences.

## Benefits

BES delivers the knowledge needed to support the President's National Energy Plan for improving the quality of life for all Americans. In addition, BES works cooperatively with other agencies and the programs of the National Nuclear Security Administration to discover knowledge and develop tools to strengthen national security. As part of its mission, the BES program plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories.

Basic research supported by the BES program touches virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. Research in materials sciences and engineering leads to the development of materials that improve the efficiency, economy, environmental acceptability,

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[a] Reflects a rescission in accordance with P.L. 109-148, the Emergency Supplemental Appropriations Act to address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006, as follows: Materials Sciences and Engineering (-$7,461,000); Chemical Sciences, Geosciences, and Energy Biosciences (-$2,218,000); and Construction (-$1,780,000).
[b] Reflects a reallocation of funding in accordance with H.Rpt. 109-86, the report for the House-passed Energy and Water Development Appropriations Act, 2006, as follows: Materials Sciences and Engineering (-$967,000); Chemical Sciences, Geosciences, and Energy Biosciences (+$967,000).
[c] Total is reduced by $8,898,000 for a rescission in accordance with P.L. 108-447, the Consolidated Appropriations Act, 2005; $18,764,000, which was transferred to the SBIR program; and $2,252,000, which was transferred to the STTR program.

and safety of energy generation, conversion, transmission, and use. For example, research on toughened ceramics will result in improved high-speed cutting tools, engine turbines, and a host of other applications requiring lightweight, high-temperature materials. Research in chemistry leads to the development of advances such as efficient combustion systems with reduced emissions of pollutants; new solar photo conversion processes; improved catalysts for the production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. Research in geosciences contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation and seismic imaging for reservoir definition. Finally, research in the molecular and biochemical nature of photosynthesis aids the development of solar photo energy conversion and biomass conversion. History has taught us that seeking answers to fundamental questions results in a diverse array of practical applications as well as some remarkable revolutionary advances.

**Strategic and Program Goals**

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

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

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

Program Goal 5.22.00.00: Advance the Basic Science for Energy Independence – Provide the scientific knowledge and tools to achieve energy independence, securing U.S. leadership and essential breakthroughs in basic energy sciences.

**Contribution to Program Goal 5.22.00.00 (Advance the Basic Science for Energy Independence)**

Within the Basic Energy Sciences program, the Materials Science and Engineering subprogram and the Chemical Sciences, Geosciences, and Energy Biosciences subprogram contribute to Program Goal 5.22.00.00 by producing seminal advances in the core disciplines of the basic energy sciences—materials sciences and engineering, chemistry, geosciences, and energy biosciences. These subprograms build leading research programs that provide world-class, peer-reviewed research results cognizant of both DOE mission needs and new scientific opportunities. Scientific discoveries at the frontiers of these disciplines impact energy resources, production, conversion, efficiency, and the mitigation of the adverse impacts of energy production and use—discoveries that will accelerate progress toward energy independence, economic growth, and a sustainable environment.

The following indicators establish specific long-term (10-year) goals in scientific advancement that the BES program is committed to and that progress can be measured against.

- Design, model, fabricate, characterize, analyze, assemble, and use a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more—particularly at the nanoscale—for energy-related applications.
- Understand, model, and control chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic and biological systems.

- Develop new concepts and improve existing methods to assure a secure energy future, e.g., for solar energy conversion and for other energy sources.
- Conceive, design, fabricate, and use new scientific instruments to characterize and ultimately control materials, especially instruments for x-ray, neutron, and electron beam scattering and for use with high magnetic and electric fields.

The Materials Science and Engineering subprogram also contributes to Program Goal 5.22.00.00 by managing BES facility operations and construction to the highest standards of overall performance, using merit evaluation with independent peer review. The synchrotron radiation light sources, neutron scattering facilities, and electron-beam micro characterization centers reveal the atomic details of metals and alloys; glasses and ceramics; semiconductors and superconductors; polymers and biomaterials; proteins and enzymes; catalysts, molecular sieves, and filters; and materials under extremes of temperature, pressure, strain, and stress. Researchers are now able to make new materials and study their atomic formation as it happens using these new probes. Once the province of specialists, mostly physicists, these facilities are now used by thousands of researchers annually from all disciplines. The Materials Science and Engineering subprogram is also establishing a suite of Nanoscale Science Research Centers that will change the way materials research is done by providing the ability to fabricate complex structures using chemical, biological, and other synthesis techniques; characterize them; assemble them; and integrate them into devices—and do it all in one place. The Chemical Sciences, Geosciences, and Energy Biosciences subprogram contribute to this goal by managing the Combustion Research Facility at Sandia National Laboratories in Livermore, California, an internationally recognized facility for advanced characterization techniques and for the study of combustion science and technology.

## Funding by General and Program Goal

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| General Goal 5, World-Class Scientific Research Capacity | | | |
| Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence (Basic Energy Science) | 1,083,616 | 1,134,557 | 1,420,980 |

## Annual Performance Results and Targets

| FY 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Program Goal 5.22.00.00 Advance the Basic Science for Energy Independence | | | | | |
| Materials Sciences and Engineering | | | | | |
| N/A | N/A | Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 100 nm and in the soft x-ray region was measured at 19 nm, and spatial information limit for an electron microscope of 0.078 nm was achieved. [Met Goal] | Improve Spatial Resolution: Spatial resolution for imaging in the hard x-ray region was measured at 90 nm and in the soft x-ray region was measured at 15 nm, and spatial information limit for an electron microscope of 0.078 nm was achieved. [Met Goal] | Improve Spatial Resolution: Demonstrate measurement of spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm.[a] | Improve Spatial Resolution: Demonstrate measurement of spatial resolutions for imaging in the hard x-ray region of <100 nm and in the soft x-ray region of <18 nm, and spatial information limit for an electron microscope of 0.08 nm.[a] |
| N/A | N/A | Improve temporal resolution: X-ray pulses were measured at 20 femtoseconds in duration with an intensity of 10,000 photons per pulse. [Met Goal] | Improve temporal resolution: X-ray pulses were measured at 70 femtoseconds in duration with an intensity of 100 million photons per pulse. [Met Goal] | Improve temporal resolution: Demonstrate measurement of x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million photons per pulse ($>10^8$ photons/pulse).[a] | Improve temporal resolution: Demonstrate measurement of x-ray pulses that are <100 femtoseconds in duration and have an intensity of >100 million photons per pulse ($>10^8$ photons/pulse).[a] |
| Chemical Sciences, Geosciences, and Energy Biosciences | | | | | |
| N/A | N/A | As a part of the Scientific Discovery through Advanced Computing (SciDAC) program, a two-dimensional combustion reacting flow simulation was performed involving 44 reacting species and 518,400 grid points. [Met Goal] | As a part of the Scientific Discovery through Advanced Computing (SciDAC) program, a three-dimensional combustion reacting flow simulation was performed involving 11 reacting species and 0.5 billion grid points. [Met Goal] | Improve Simulation: Perform a three-dimensional combustion reacting flow simulation involving more than 30 reacting species and 20 million grid points. | Improve Simulation: Beginning in FY 2007, increasing the size of the simulation will no longer provide useful new information. Thus, this measure is being discontinued. |
| Materials Sciences and Engineering | | | | | |
| Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time. [Met Goal] | Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time. [Met Goal] | Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time (Results: 91.9%). [Met Goal] | Scientific user facilities were maintained and operated to achieve an average at least 90% of the total scheduled operating time (Results: 97.7%). [Met Goal] | Maintain and operate the scientific user facilities to achieve an average at least 90% of the total scheduled operating time. | Maintain and operate the scientific user facilities to achieve an average at least 90% of the total scheduled operating time. |

[a] No further improvement is expected in FY 2006–FY 2011 as compared to the level of achievement for FY 2005. Performance levels for resolution (temporal and spatial) have reached the maximum for the current suite of available instruments. This target is a measure of SC's intent to maintain the maximum level of performance for users of the current SC facilities until the next generation of instruments and facilities becomes available.

| FY 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Construction | | | | | |
| Cost and timetables were maintained within 10% of the baselines given in the construction project data sheets for all construction projects ongoing during the year. [Met Goal] | Cost and timetables were maintained within 10% of the baselines given in the construction project data sheets for all construction projects ongoing during the year. [Met Goal] | Cost and timetables were maintained within 10% of the baselines given in the construction project data sheets for all construction projects ongoing during the year (Results: +1.3% cost variance and +0.8% schedule variance). [Met Goal] | Cost and timetables were maintained within 10% of the baselines given in the construction project data sheets for all construction projects ongoing during the year (Results: +0.2% cost variance and -2.5% schedule variance). [Met Goal] | Meet the cost and timetables within 10% of the baselines given in the construction project data sheets for all ongoing construction projects. | Meet the cost and timetables within 10% of the baselines given in the construction project data sheets for all ongoing construction projects. |


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## Means and Strategies

The Basic Energy Sciences program will use various means and strategies to achieve its program goals. However, various external factors may impact the ability to achieve these goals.

The BES program will support fundamental, innovative, peer-reviewed research to create new knowledge in areas important to the BES mission, i.e., in materials sciences and engineering, chemical sciences, geosciences, and biosciences. BES also plays a critical role in constructing and operating a wide array of scientific user facilities for the Nation's researchers. All research projects undergo regular peer review and merit evaluation based on procedures set down in 10 CFR 605 for the extramural grant program and under a similar process for the laboratory programs and scientific user facilities. All new projects are selected through peer review and merit evaluation.

External factors, in addition to budgetary constraints, that affect the level of performance include: (1) changing mission needs as described by the DOE and SC mission statements and strategic plans; (2) scientific opportunities as determined, in part, by proposal pressure and scientific workshops; (3) the results of external program reviews and international benchmarking activities of entire fields or sub-fields, such as those performed by the National Academy of Sciences; (4) unanticipated failures in critical components of scientific user facilities or major research programs; and (5) strategic and programmatic decisions made by non-DOE funded domestic research activities and by major international research centers.

The BES program in fundamental science is closely coordinated with the activities of other federal agencies (e.g., National Science Foundation, National Aeronautics and Space Administration, Department of Agriculture, Department of Interior, and National Institutes of Health). BES also promotes the transfer of the results of its basic research to contribute to DOE missions in areas of energy efficiency, renewable energy resources, improved use of fossil fuels, nuclear energy, reduced environmental impacts of energy production and use, national security, and future energy sources.

## Validation and Verification

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

## Program Assessment Rating Tool (PART)

The Department implemented a tool to evaluate selected programs. PART was developed by OMB to provide a standardized way to assess the effectiveness of the Federal Government’s portfolio of programs. The structured framework of the PART provides a means by which programs can assess their activities differently than by traditional reviews. The BES program has incorporated feedback from OMB and has taken the necessary steps to continue to improve performance.

In the FY 2005 PART review, OMB gave the BES program a very high score of 93% overall which corresponds to a rating of “Effective.” OMB found the program to be strategically driven and well managed. Outside expert panels have validated the program’s merit-based review processes ensuring that research supported is relevant and of very high quality. The assessment found that BES has developed a limited number of adequate performance measures which are continued for FY 2007. These measures have been incorporated into this Budget Request, BES grant solicitations, and the performance plans of senior managers. As appropriate, they will be incorporated into the performance based contracts of M&O contractors. To better explain our scientific performance measures, the Office of Science developed a website (http://www.sc.doe.gov/measures) that answers questions such as "What does this measure mean?" and "Why is it important?" Roadmaps, developed in consultation with the Basic Energy Sciences Advisory Committee (BESAC), will guide triennial reviews by BESAC of progress toward achieving the long term Performance Measures. These roadmaps are posted on the SC website. The Annual Performance Targets are tracked through the Department's Joule system and reported in the Department's Annual Performance Report.

OMB developed PARTWeb for the FY 2007 Budget—a new interface for PART that facilitates collaboration between agencies and OMB. PARTWeb will link to the website http://ExpectMore.gov and will improve public access to PART assessments and follow up actions. For 2006, there are three continuing actions and one new action for Basic Energy Sciences.

- Following up on recommendations of past expert reviews, and using new reviews to assess progress toward long-term programmatic goals.
- The Department will work to include the long-term goals of each program in grant solicitations, and will improve performance reporting by grantees and contractors.
- Improving performance reporting at its user facilities to better reflect the instrumentation and staffing issues most directly connected to scientific output.
- New action—producing a detailed corporate solution for managing and operating the High Flux Isotope Reactor that explicitly addresses the reliability problems while ensuring public health and safety.

In response, BES will continue to use the Committees of Visitors to review progress toward the long term goals of the program and will continue efforts to improve performance reporting. A review of the management and operations of the High Flux Isotope Reactor has been scheduled in 2006 that will address reliability, safety, and health issues. The solution to the reliability problem will be contained in the Basic Energy Sciences report of the review results.

**Overview**

BES and its predecessor organizations have supported a program of fundamental research focused on critical mission needs of the Nation for over five decades. The federal program that became BES began with a research effort initiated to help defend our Nation during World War II. The diversified program was organized into the Division of Research with the establishment of the Atomic Energy Commission in 1946 and was later renamed Basic Energy Sciences as it continued to evolve through legislation included in the Atomic Energy Act of 1954, the Energy Reorganization Act of 1974, the Department of Energy Organization Act of 1977, and the Energy Policy Act of 1992.

Today, the BES program is one of the Nation's largest sponsors of research in the natural sciences. It is uniquely responsible for supporting fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences impacting energy resources, production, conversion, and efficiency, and the mitigation of the adverse impacts of energy production and use. In FY 2005, the program funded research in more than 190 academic institutions located in 48 states and in 13 Department of Energy (DOE) laboratories located in 9 states. BES supports a large extramural research program, with approximately 35% of the program's research activities sited at academic institutions.

The BES program also supports world-class scientific user facilities, providing outstanding capabilities for imaging and characterizing materials of all kinds from metals, alloys, and ceramics to fragile biological samples. The BES synchrotron radiation light sources, the neutron scattering facilities, and the electron beam characterization centers represent the largest and best collection of such facilities supported by a single organization in the world. Annually, 8,000 researchers from universities, national laboratories, and industrial laboratories perform experiments at these facilities. Spurred by results of past investments and by innovations in accelerator concepts, the BES program continues its pioneering role in the development of new generations of scientific research instruments and facilities.

The 2001 "National Energy Policy" noted that the U.S. economy grew by 126% since 1973, but energy use increased by only 30%. Approximately one-half to two-thirds of the savings resulted from technological improvements in products and services that allow consumers to enjoy more energy services without commensurate increases in energy demand. At the heart of these improvements is fundamental research. During this 30-year period, the basic research supported by the BES program has touched virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. The basic knowledge derived from fundamental research has resulted in a vast array of advances, including:

- high-energy and high-power lithium and lithium ion batteries and thin-film rechargeable micro batteries;
- thermo acoustic refrigeration devices that cool without moving parts and without the use of freons;
- compound semiconductors, leading to the world's highest efficiency photovoltaic solar cells;
- catalysts for the production of new polymers (annually, a multibillion dollar industry) and for a host of other products and energy-efficient processes;
- high-strength, lightweight magnets for sensors and for small motors used in power steering and other vehicle functions;
- strong, ductile alloys for use in high-temperature applications;
- nonbrittle ceramics for use in hammers, high-speed cutting tools, engine turbines, and other applications requiring lightweight and/or high-temperature materials;
- new steels, improved aluminum alloys, magnet materials, and other alloys;
- polymer materials for rechargeable batteries, car bumpers, food wrappings, flat-panel displays, wear-resistant plastic parts, and polymer-coated particles in lubricating oils; and
- processes for extraction of radioactive and hazardous metal ions from solutions for nuclear fuel purification/reprocessing and for cleanup of radioactive wastes.

These advances came by exploiting the results of basic research that sought answers to the most fundamental questions in materials sciences, chemistry, and the other disciplines supported by BES.

The future holds even greater promise, largely because of our new atom-by-atom understanding of matter and the subsequent unprecedented ability to design and construct new materials with properties that are not found in nature. This understanding comes in large measure from synchrotron x-ray and neutron scattering sources, electron microscopes, and other atomic probes as well as terascale computers. The BES program has played a major role in enabling the nanoscale revolution. This impact results from a deliberate philosophy of identifying seminal challenges and establishing both facilities and coordinated programs that transcend what individuals alone can do. The program in nanoscale science, including the formation of Nanoscale Science Research Centers, continues that philosophy.

### How We Work

To ensure that the most scientifically promising research is supported the BES program engages in long-range planning and prioritization; regular external, independent review of the supported research to ensure quality and relevance; and evaluation of program performance through establishment and subsequent measurement against goals and objectives. These activities rely heavily on input from external sources including workshops and meetings of the scientific community, advice from the federally chartered Basic Energy Sciences Advisory Committee (BESAC), intra-DOE and Interagency Working Groups, and reports from other groups such as the National Academy of Sciences. To accomplish its mission, the BES program supports research in both universities and DOE laboratories; plans, constructs, and operates world-class scientific user facilities; and maintains a strong infrastructure to support research in areas of core competencies. Some of the details of how we work are given in the sections below.

**Advisory and Consultative Activities**

Charges are provided to BESAC by the Director of the Office of Science. During the past few years, BESAC has provided advice on new directions in nanoscale science and complex systems; on the operation of the major scientific user facilities; on the need for new, "next-generation" facilities for x-ray, neutron, and electron-beam scattering; on performance measurement; on the quality of the BES program management and its consequent impacts on the program portfolio; on new directions in research relating to specific aspects of fundamental science such as catalysis, biomolecular materials, and computational modeling at the nanoscale; on the fundamental research challenges posed by the Department's energy missions; on a 20-year roadmap for BES facilities; and on theory and computation needs across the entire portfolio of BES research. Of particular note is the BESAC report "Basic Research Needs to Assure a Secure Energy Future," which describes 10 themes and 37 specific research directions for increased emphasis. This report will help the program map its research activities for many years to come.

Information and reports for all of the above mentioned advisory and consultative activities are available on the BESAC website (http://www.science.doe.gov/production/bes/BESAC/BESAC.htm). Other studies are commissioned as needed using the National Academy of Science's National Research Council and other independent groups.

**Facility Reviews**

Facilities are reviewed using (1) external, independent review committees operating according to the procedures established for peer review of BES laboratory programs and facilities (http://www.science.doe.gov/bes/labreview.html) and (2) specially empanelled subcommittees of BESAC. These subcommittees have reviewed the synchrotron radiation light sources, the neutron scattering facilities, and the electron-beam micro characterization facilities. The reports of these reviews are available on the BES website (http://www.science.doe.gov/bes/BESAC/reports.html). Regardless of whether a review is by an independent committee charged by a BES program manager or by a BESAC subcommittee charged by the Director of the Office of Science, the review has standard elements. Important aspects of the reviews include assessments of the quality of research performed at the facility; the reliability and availability of the facility; user access policies and procedures; user satisfaction; facility staffing levels; R&D activities to advance the facility; management of the facility; and long-range goals of the facility.

These reviews have identified both best practices and substantive issues, including those associated with mature facilities. For example, the reviews clearly highlighted the change that occurred as the light sources transitioned from a mode in which they served primarily expert users to one in which they served very large numbers of inexperienced users in a wide variety of disciplines. The light sources experienced a quadrupling of the number of users in the decade of the 1990s. This success and its consequent growing pains were delineated by our reviews. The outcomes of these reviews helped develop new models of operation for existing light sources and neutron scattering facilities as well as the new Spallation Neutron Source now under construction.

Facilities that are in design or construction are reviewed according to procedures set down in DOE Order 413.3 "Program and Project Management for Capital Assets" and in the Office of Science "Independent Review Handbook" (http://www.science.doe.gov/opa/PDF/revhndbk.pdf). In general, once a project has entered the construction phase (e.g., the Spallation Neutron Source, the Linac Coherent Light Source, or the Nanoscale Science Research Centers), it is reviewed with external, independent committees approximately biannually. These Office of Science construction project reviews enlist experts in the technical scope of the facility under construction and its costing, scheduling, and construction management.

**Program Reviews**

All research projects supported by the BES program undergo regular peer review and merit evaluation based on procedures set down in 10 CFR Part 605 for the extramural grant program and in an analogous process for the laboratory programs (http://www.science.doe.gov/bes/labreview.html). These peer review and merit evaluation procedures are described within documents found at http://www.science.doe.gov/bes/peerreview.html. These evaluations assess:

(1) Scientific and/or technical merit or the educational benefits of the project;
(2) Appropriateness of the proposed method or approach;
(3) Competency of personnel and adequacy of proposed resources;
(4) Reasonableness and appropriateness of the proposed budget; and
(5) Other appropriate factors, established and set forth by SC in a notice of availability or in a specific solicitation.

In addition, on a rotating schedule, BESAC reviews the major elements of the BES program using Committees of Visitors (COVs). COVs are charged with assessing the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document proposal actions; the quality of the resulting portfolio, specifically the breadth and depth of portfolio elements and the national and international standing of the elements; and progress toward the long-term PART goals. The first three reviews assessed the chemistry activities (FY 2002), the materials sciences and engineering activities (FY 2003), and the activities associated with the management of the light sources, the neutron sources, and the new Nanoscale Science Research Centers (FY 2004). This COV review cycle began again in FY 2005, so that all elements of the BES program are reviewed every three years.

**Planning and Priority Setting**

Because the BES program supports research covering a wide range of scientific disciplines as well as a large number of major scientific user facilities, planning is an ongoing activity. Many long-range planning exercises for elements of the BES program are performed under the auspices of BESAC. Prioritization within each of these program elements is achieved via such studies. Prioritization across the entirety of the BES program is more complex than that for a homogeneous program where a single planning exercise results in a prioritization.

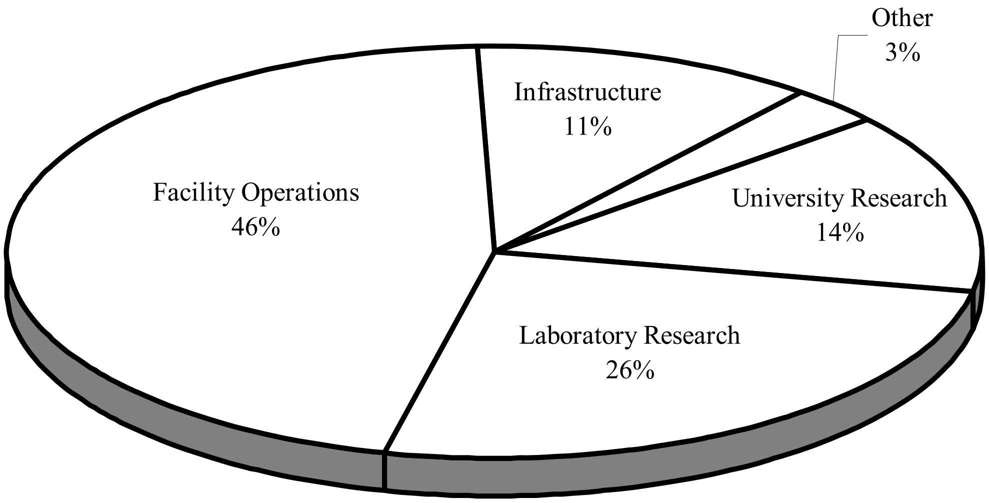
Inputs to our prioritization include overall scientific opportunity, projected investment opportunity, DOE mission need, and Administration and Departmental priorities. During the past few years, these considerations have led to: increased investments in science at the nanoscale to take advantage of the remarkable knowledge gained from atomic-scale understanding of materials; increased investments for operations of the major user facilities in recognition of the quadrupling of users in the past decade and to reap the rewards of the capital investments in the facilities themselves; increased investments for instrumentation at the facilities so that the quality of the instruments will match the world-class quality of the facilities; increased investments for ultrafast science to probe processes that happen on the timescale of chemical reactions; and increases for targeted program areas for which both scientific opportunity and mission need are high (e.g., basic research for the hydrogen economy and basic research for effective solar energy utilization) or for which BES represents the sole U.S. steward of the field (e.g., heavy-element chemistry). Construction of new user facilities such as the Spallation Neutron Source, the Linac Coherent Light Source, the Nanoscale Science Research Centers, or upgrades or replacements to existing facilities such as the High Flux Isotope Reactor, the Stanford Synchrotron Radiation Laboratory, and the National Synchrotron Light Source-II follow from input from BESAC and National Academy of Sciences studies and from broad, national strategies that include the input from multiple federal agencies.

The FY 2007 budget request continues priorities established in the past few years. The Spallation Neutron Source will enter its first year of full operation after construction from FY 1999 to FY 2006. A significant investment in the area of nanoscale science includes the operation of new Nanoscale Science Research Centers at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, Argonne National Laboratory and Sandia National Laboratories/Los Alamos National Laboratory. Construction funding is provided for the Nanoscale Science Research Center at Brookhaven National Laboratory. Project Engineering Design and construction funding also are provided for the Linac Coherent Light Source (LCLS), a 4$^{th}$ generation light source that will provide orders of magnitude higher intensities of coherent x-ray light than do current synchrotron radiation light sources. The LCLS will be a facility for groundbreaking research in the physical and life sciences owing to its femtosecond pulses of extremely high peak brightness x-ray beams. It will be the first such facility in the world. R&D funding is provided for upgrades on next-generation x-ray synchrotron and spallation neutron sources.

**How We Spend Our Budget**

The BES program has three major program elements: research, facility operations, and construction and laboratory infrastructure support. Approximately 35% of the research funding goes to support work in universities with most of the remainder going to support work in DOE laboratories. The facility operations budget has grown relative to the research budget over the past decade, reflecting the commissioning of new and upgraded facilities as well as the increased importance of these facilities in enabling the research of thousands of researchers across the Nation. Project Engineering Design (PED) and construction funding remain significant budget components in FY 2007 for the Linac Coherent Light Source, the Nanoscale Science Research Center at Brookhaven National Laboratory, and the National Synchrotron Light Source-II. The FY 2007 Request also includes construction funding for the Advanced Light Source (ALS) User Support Building at the Lawrence Berkeley National Laboratory.

## Basic Energy Sciences Budget Allocation
## FY 2007




**Research**

The BES program is one of the Nation's largest supporters of fundamental research. Research is supported in both DOE laboratories and universities. While peer review of all research ensures outstanding quality and relevance, each of the two research sectors has unique characteristics and strengths.

National Laboratory Research: Research sited at DOE laboratories often takes advantage of the premier scientific user facilities for x-ray, neutron, and electron beam scattering at the laboratories as well as other specialized facilities, such as hot cells, which are not typically found at universities. Mission critical research is also sited at DOE laboratories when it is outside of the mainstream of research supported at universities, e.g., heavy-element chemistry or combustion chemistry. Research sited at DOE laboratories is very often collocated with and sometimes cofunded with research activities of the DOE technology offices, providing a synergism not available in universities. Finally, research that requires strong interdisciplinary interactions, large teams of closely collaborating researchers, or a large technical support staff is also well suited to DOE laboratories.

University Research: Universities provide access to the Nation's largest scientific talent pool and to the next-generation of scientists. Development of the workforce through the support of faculty, graduate students working toward a doctoral degree, and postdoctoral associates developing their research and management skills is a high priority. The R&D workforce developed under this program provides new scientific talent in areas of fundamental research. Furthermore, engaging faculty and students in the work of the BES program develops a broad appreciation for the basic research needs associated with the program.

Collaborations between National Laboratory Research and University Research: Historically, collaborations between the two research sectors have been strong, particularly in areas where both sectors derive significant benefits. Examples include the use of the major BES facilities by university and industry researchers and the contribution of these researchers to new instrument concepts and to instrument fabrication at the facilities. The Nanoscale Science Research Centers and new activities in ultrafast science and basic research for the hydrogen economy are expected to both strengthen and broaden these partnerships.

**Significant Program Shifts**

In FY 2007, there are a number of significant program milestones and increases, including the following in the area of construction and Major Items of Equipment:

- Construction of the Spallation Neutron Source (SNS) will be completed during the 3rd quarter of FY 2006. Over the next two to three years, the facility will continue to fabricate and commission instruments, funded both as part of the SNS project and from other sources including non-DOE sources, and will increase power to full levels. A new Major Item of Equipment is funded in FY 2007 that will allow the fabrication of approximately four to five additional instruments for the SNS, thus nearly completing the initial suite of 24 instruments that can be accommodated in the high-power target station ($10,000,000).
- Four Nanoscale Science Research Centers will be fully operational in FY 2007: the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, the Molecular Foundry at Lawrence Berkeley National Laboratory, the Center for Nanoscale Materials at Argonne National Laboratory, and the Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory. A fifth Center, the Center for Functional Nanomaterials at Brookhaven National Laboratory, will receive final year construction funding.
- The Linac Coherent Light Source will continue Project Engineering Design (PED) and construction at the planned levels. Funding is provided separately for preconceptual design and fabrication of instruments for the facility. Funding is also provided to partially support operation of the SLAC linac. This marks the second year of the transition to LCLS operations at SLAC.
- Support is provided for PED ($20,000,000) and Other Project Costs ($25,000,000) for the National Synchrotron Light Source-II (NSLS-II), which will be built as a replacement for NSLS-I, to enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. NSLS-II will provide the world's finest capabilities for x-ray imaging.
- Support is provided for PED for the Advanced Light Source User Support Building ($3,000,000), which will provide space for experimental set up of equipment prior to use at the Advanced Light Source, space to accommodate a long beam line that will extend from the floor of the Advanced Light Source into the User Support Building, and temporary office space and conference rooms for users.

There also are a number of increases in research. In FY 2007, the Office of Science will support expanded efforts in basic research related to transformational energy technologies. This derives from the BESAC workshop report "Basic Research Needs to Assure a Secure Energy Future." Within BES, there are increases to ongoing basic research for effective solar energy utilization, for the hydrogen economy, and for work underpinning advanced nuclear energy power. These are described briefly below. BES not only asks its communities of scientists to provide the scientific foundations to overcome short-term "showstoppers" in energy technologies such as these three, BES also asks researchers to reach far beyond today's problems in order to provide the basis for long-term solutions to what is probably society's greatest challenge—a secure, abundant, and clean energy supply. To that end, there also are increases in research for grand challenge science questions and for new technique development. Grand challenge science includes the study of the fundamental phases of matter and phase transitions; quasiparticles; interactions of strong and weak forces in molecular bonding; "communication" among electrons, atoms, molecules, cells, and organisms; the harnessing of properties of elementary particles, atoms, and molecules to create fundamentally new ways to store, manipulate, and transmit information; and organizing principles at the nanoscopic and mesoscopic scales, intermediate between atomic and macroscopic dimensions. This will be a topic of a forthcoming BESAC workshop.

Briefly, additional research funding is provided in the following areas:

- Basic research for the hydrogen economy. Research to realize the potential of a hydrogen economy will be increased from $32,500,000 to $50,000,000. The research program is based on the BES workshop report "Basic Research Needs for the Hydrogen Economy." The results of the FY 2005 solicitation are described later in this document.
- Basic research for effective solar energy utilization (+$34,115,000). Investments will be focused in three areas: solar-to-electric, solar-to-fuels, and solar-to-thermal conversions. Each of the three generic approaches to exploiting the solar resource has untapped capability well beyond its present usage. Many of the proposed research directions identified in the 2005 BES workshop report "Basic Research Needs for Solar Energy Utilization" concern important cross-cutting issues such as (1) coaxing cheap materials to perform as well as expensive materials in terms of their electrical, optical, chemical, and physical properties (e.g., polycrystalline materials versus expensive single crystal materials or plastics and polymers instead of metals and semiconductors); (2) developing new paradigms for solar cell design that surpass traditional efficiency limits; (3) finding catalysts that enable inexpensive, efficient conversion of solar energy into chemical fuels; (4) identifying novel methods for self-assembly of molecular components into functionally integrated systems; and (5) developing materials for solar energy conversion infrastructure, such as transparent conductors and robust, inexpensive thermal management materials. Powerful new methods of nanoscale fabrication, characterization, and simulation—using tools that were not available as little as five years ago—create new opportunities for understanding and manipulating the molecular and electronic pathways of solar energy conversion.
- Basic research for advanced nuclear energy systems (+$12,432,000). Basic research related to advanced fuel cycles is needed in areas such as (1) control and predictive capability of processes driven by small energy differences, e.g., aggregation and precipitation; (2) fundamental principles to guide ligand design; (3) investigation of new separations approaches based on magnetic and electronic differences; (4) development of environmentally benign separations processes, which produce no secondary wastes and consume no chemicals; and (5) development of modeling of separations processes to optimize waste minimization and minimize opportunities for diversion of nuclear materials (i.e. optimize proliferation resistance). Basic research also is needed in areas of materials for advanced reactors and waste forms for spent fuels from the new generation of reactors. This requires understanding and predicting the properties and behaviors of materials over long time scales and multiple length scales—from atoms to bulk materials. The efficiency, safe operating lifetime, and overall performance of fission energy systems is limited by the load-bearing capacity of structural materials under the maximum temperatures and hostile corrosive, applied stress, and radiation environmental parameters under which they must perform. New generation fission systems require structural materials possessing a combination of properties that will enable them to sustain their performance under such hostile parameters for durations of the order of 100 years.
- Complex systems or emergent behavior (+$5,000,000). Emergent behaviors arise from the collective, cooperative behavior of individual components of a system. Current understanding of emergent behaviors is very limited. The challenge of understanding how emergent behavior results from the complexity of competing interactions is among the most compelling of our time, spanning

physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magneto resistance, random field magnets, and spin liquids and glasses. Investments will encompass experimental, theoretical, and computational approaches capable of interrogating systems at comparable physical and time scales to gain direct insight into the mechanisms underpinning the cooperative behavior. Unlocking the mysteries of these systems will lay the scientific foundation for designing and engineering new multifunctional materials, devices and sensors with exquisitely sensitive properties.

- Ultrafast science (+$10,000,000). Ultrafast science deals with physical phenomena that occur in the range of one-trillionth of a second (one picosecond) to less than one-quadrillionth of a second (one femtosecond). These phenomena are typically probed using extremely short pulses of coherent light from conventional lasers or free electron lasers such as the Linac Coherent Light Source. Ultrafast technology has applications across the fields of atomic and molecular physics, chemistry and chemical biology, coherent control of chemical reactions, materials sciences, magnetic- and electric-field phenomena, optics, and laser engineering. Examples include the making and breaking of molecular bonds and the observation of the elusive chemical transition state. New investments in ultrafast science will focus on research applications of x-ray sources associated with BES facilities and beamlines: the Linac Coherent Light Source; the femtosecond "slicing" beamline at the Advanced Light Source; and the short pulse development at the Advanced Photon Source. Investments will also be made in the development and applications of laser-driven, table-top x-ray sources, including the use of high-harmonic generation to create bursts of x-rays on the even shorter than the femtosecond time scale.
- Mid-scale instrumentation (+$10,000,000). Scientific progress is predicated on observations of new phenomena, which often involve the building of better tools. There is a significant national need for mid-scale instruments that serve multiple users yet which are not as large as the synchrotron and neutron sources. High priority mid-scale instrumentation needs include end stations at the synchrotron light sources and neutron scattering facilities; laser systems for ultrafast or high-energy-density studies; micro- and atomic-scale characterization tools such as electron microcharacterization and scanning probe microscopy; high-field magnets; and facilities for providing large crystals and other unique materials for researchers throughout the Nation.
- Chemical imaging (+$5,000,000). Investments will develop and apply new methods to measure the chemical behavior of individual molecules and reactions, with high resolution in both space and time in order to elucidate fundamental principles of chemical processes at the nanoscale level. The research will build on current single-molecule spectroscopies and microscopies by adding simultaneous time-dependent characterization of evolving chemical processes, ultimately with femtosecond time resolution.

Additional information on these activities is in the relevant Construction Project Data Sheets and throughout the detailed narrative justifications.

In FY 2007, there are significant shifts in the nanoscale science and engineering research activities contributing to the BES investments in research at the nanoscale and a substantial overall increase in funding. Four of the five planned Nanoscale Science Research Centers are in their first full year of operation, with only one Center still in construction. Overall, the total investment for these Nanoscale Science Research Centers decreases by about 10 percent owing to the planned decrease in construction funding. Funding for research at the nanoscale increases very significantly owing to increases in funding for activities related to the hydrogen economy, solar energy conversion, advanced nuclear energy systems, fundamental studies of materials at the nanoscale, and instrumentation for characterizing materials at the nanoscale.

## Nanoscale Science Research Funding

(dollars in thousands)

| | TEC | TPC | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|---|---|
| Materials Sciences and Engineering | | | | | |
| Research | | | 65,307 | 70,328 | 108,542 |
| Major Item of Equipment, Center for Nanophase Materials (ANL) | | | 12,000 | 14,000 | — |
| Facility Operations | | | | | |
| Center for Functional Nanomaterials (BNL) | | | — | — | — |
| Center for Integrated Nanotechnologies (SNL/A & LANL) | | | — | 11,900 | 19,190 |
| ORNL, Center for Nanophase Materials Sciences | | | — | 17,800 | 19,190 |
| Center for Nanophase Materials (ANL) | | | — | 3,500 | 19,190 |
| Molecular Foundry (LBNL) | | | — | 8,100 | 19,190 |
| Chemical Sciences, Geosciences, and Biosciences | | | | | |
| Research | | | 27,645 | 26,914 | 49,109 |
| Project Engineering Design and Construction | | | | | |
| PED– All sites | | 21,318 | 1,996 | — | — |
| Construction | | | | | |
| Center for Functional Nanomaterials (BNL) | 79,700 | 81,000 | 18,317 | 36,187 | 18,864 |
| Center for Integrated Nanotechnologies (SNL/A & LANL) | 73,754 | 75,754 | 30,650 | 4,580 | 247 |
| ORNL, Center for Nanophase Materials Sciences | 63,740 | 64,740 | 17,669 | — | — |
| Molecular Foundry (LBNL) | 83,604 | 84,904 | 31,828 | 9,510 | 257 |
| Total | | | 205,412 | 202,819 | 253,779 |

In FY 2007, $50,000,000 is requested for basic research activities to realize the potential of a hydrogen economy. The research program is based on the BES workshop report “Basic Research Needs for the Hydrogen Economy” that can be found at http://www.science.doe.gov/production/bes/hydrogen.pdf. The 2003 report highlights the enormous gap between our present capabilities for hydrogen production, storage, and use and those required for a competitive hydrogen economy. To be economically competitive with the present fossil fuel economy, the cost of fuel cells must be lowered by a factor of five and the cost of producing hydrogen must be lowered by a factor of four. Moreover, the performance and reliability of hydrogen technology for transportation and other uses must be improved dramatically. Simple incremental advances in the present state-of-the-art cannot bridge this gap. Narrowing the gap significantly will require a comprehensive, long-range program of innovative high-risk/high-payoff basic research that is intimately coupled to and coordinated with applied programs. The objective of such a program must not be evolutionary advances but rather revolutionary breakthroughs in understanding and in controlling the chemical and physical interactions of hydrogen with materials. Detailed findings and research directions identified by the three panels are presented in the report.

In response to the BES solicitation on Basic Research for the Hydrogen Fuel Initiative for FY 2005 funding, 668 qualified preapplications were received in five submission categories: (1) novel materials for hydrogen storage, (2) membranes for separation, purification, and ion transport, (3) design of catalysts at the nanoscale, (4) solar hydrogen production, and (5) bio-inspired materials and processes. Three of the five focus areas—novel storage materials, membranes, and design of catalysts at the nanoscale—accounted for about 75% of the submissions. Following a review, principal investigators on about 40% of the preapplications were invited to submit full applications; 227 full applications were received and were peer reviewed according to the guidelines in 10 CFR 605; 70 awards were made in late FY 2005. BES involved staff from EERE in the preapplication review process to ensure basic research relevance to technology program goals. Furthermore, BES will participate in EERE's annual program review meeting to promote information sharing and, beginning in FY 2006, will organize parallel sessions at that meeting for the BES principal investigators. A total of $21,473,000 in new funding related to the hydrogen economy was awarded in FY 2005 as a result of this solicitation. The additional $17,500,000 in FY 2007 will be used to augment awards made in FY 2005 and to fund additional proposals based on a new solicitation.

## President's Hydrogen Initiative

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Materials Sciences and Engineering Research | 14,761 | 16,600 | 28,075 |
| Chemical Sciences, Geosciences, and Biosciences | 14,422 | 15,900 | 21,925 |
| Total Hydrogen Initiative | 29,183 | 32,500 | 50,000 |

### Scientific Discovery through Advanced Computing

The Scientific Discovery through Advanced Computing (SciDAC) program is a set of coordinated investments across all Office of Science mission areas with the goal of achieving breakthrough scientific advances via computer simulation that were impossible using theoretical or laboratory studies alone. The power of computers and networks is increasing exponentially. Advances in high-end computing technology, together with innovative algorithms and software, are being exploited as intrinsic tools for scientific discovery. SciDAC has also pioneered an effective new model of multidisciplinary collaboration among discipline-specific scientists, computer scientists, computational scientists, and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can productively exploit terascale computing and networking resources. The program is bringing computation and simulation to parity with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate modeling and prediction, plasma physics, particle physics, accelerator design, astrophysics, chemically reacting flows, and computational nanoscience.

The SciDAC program in BES consists of two major activities: (1) characterizing chemically reacting flows as exemplified by combustion and (2) achieving scalability in the first-principles calculation of molecular properties, including chemical reaction rates. In the characterization of chemically reacting flows, the scientific problem is one of multiple scales from the molecular scale where the physical descriptions are discrete in nature to the laboratory scale where the physical descriptions are continuous. The method of choice for the complete characterization of combustion at all scales is direct numerical simulation. A collaboration involving Sandia National Laboratories and four universities successfully implemented a fully parallel implementation of direct numerical simulation that incorporated a widely used program for solving the species profiles for combustion systems involving dozens of species and hundreds of reactions. In achieving scalability in the first-principles calculation of molecular properties, progress has been made on several fronts, but perhaps the most encouraging is work in dealing with the problem of electron correlation, a problem responsible for the poor scaling of quantum chemistry codes. A novel method for incorporating correlation directly into quantum mechanical descriptions of atoms and molecules is now being incorporated into a massively parallel code.

**Scientific Facilities Utilization**

The BES program request supports the scientific user facilities. Research communities that have benefited from these facilities include materials sciences, condensed matter physics, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, medical research, and industrial technology development. More detailed descriptions of the specific facilities and their funding are given in the subprogram narratives and in the sections entitled Site Description and Major User Facilities.

Two tables follow: The first shows the hours of operation and numbers of users for the major scientific user facilities—the synchrotron radiation sources and the neutron scattering facilities. The second shows cost and schedule variance. Note: Cost Variance is the difference between the value of the physical work performed and the actual cost expended. A negative result is unfavorable and indicates the potential for a cost overrun. Schedule variance is the difference between the value of the physical work performed and the value of the work planned. A negative result is unfavorable and indicates that the project is behind schedule. Variance data are shown as percents. They are shown against the project's performance measurement baseline that includes cost and schedule contingency and are as of the end of each fiscal year. All projects have met or are on schedule to meet all Level 0 and Level 1 Milestones, which are shown in the table.

## Synchrotron Light Source and Neutron Scattering Facility Operations

| | FY 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| All Facilities | | | |
| Optimal Hours[a] | 30,700 | 31,300 | 32,700 |
| Scheduled Hours[b] | 28,129 | 30,610 | 32,700 |
| Unscheduled Downtime | 7.9% | <10% | <10% |
| Number of Users | 9,042 | 8,050 | 9,660 |
| Advanced Light Source | | | |
| Optimal Hours[a] | 5,600 | 5,600 | 5,600 |
| Scheduled Hours[b] | 5,344 | 5,520 | 5,600 |
| Unscheduled Downtime | 3.6% | <10% | <10% |
| Number of Users | 2,003 | 1,770 | 2,100 |
| Advanced Photon Source | | | |
| Optimal Hours[a] | 5,000 | 5,000 | 5,000 |
| Scheduled Hours[b] | 4,931 | 4,900 | 5,000 |

[a] Optimal hours represent the total number of hours the facilities can operate for users, which excludes routine maintenance, machine research, operator training, accelerator physics, etc. In addition, scheduled upgrades and known shutdowns for the specified fiscal year are taken into consideration. A difference between optimal hours and scheduled hours reflects a reduction in operating hours due to funding limitations.
[b] Scheduled hours for FY 2005 show actual number of hours delivered to users.

| | FY 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| Unscheduled Downtime | 1.4% | <10% | <10% |
| Number of Users | 3,215 | 2,640 | 3,300 |
| National Synchrotron Light Source | | | |
| Optimal Hours[a] | 5,500 | 5,400 | 5,400 |
| Scheduled Hours[b] | 5,313 | 5,030 | 5,400 |
| Unscheduled Downtime | 2.4% | <10% | <10% |
| Number of Users | 2,256 | 2,070 | 2,300 |
| Stanford Synchrotron Radiation Laboratory | | | |
| Optimal Hours[a] | 3,700 | 5,000 | 5,000 |
| Scheduled Hours[b] | 3,527 | 4,900 | 5,000 |
| Unscheduled Downtime | 5.0% | <10% | <10% |
| Number of Users | 1,007 | 980 | 1,200 |
| High Flux Isotope Reactor | | | |
| Optimal Hours[a] | 3,400 | 2,400 | 4,500 |
| Scheduled Hours[b] | 2,613 | 2,360 | 4,500 |
| Unscheduled Downtime | 23.2% | <10% | <10% |
| Number of Users | 96 | 100 | 220 |
| Intense Pulsed Neutron Source | | | |
| Optimal Hours[a] | 3,600 | 3,600 | 3,600 |
| Scheduled Hours[b] | 3,462 | 3,600 | 3,600 |
| Unscheduled Downtime | 4.5% | <10% | <10% |
| Number of Users | 244 | 240 | 240 |
| Manuel Lujan, Jr. Neutron Scattering Center | | | |
| Optimal Hours[a] | 3,900 | 4,300 | 3,600 |
| Scheduled Hours[b] | 2,939 | 4,300 | 3,600 |
| Unscheduled Downtime | 23.2% | <10% | <10% |
| Number of Users | 221 | 250 | 300 |
| Spallation Neutron Source[c] | | | |

[a] Optimal hours represent the total number of hours the facilities can operate for users, which excludes routine maintenance, machine research, operator training, accelerator physics, etc. In addition, scheduled upgrades and known shutdowns for the specified fiscal year are taken into consideration. A difference between optimal hours and scheduled hours reflects a reduction in operating hours due to funding limitations.
[b] Scheduled hours for FY 2005 show actual number of hours delivered to users.
[c] For the Spallation Neutron Source, there is an inadequate basis for making a reliable estimate at this time.

## Cost and Schedule Variance

| | FY 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| Spallation Neutron Source | | | |
| Cost Variance | 0% | | |
| Schedule Variance | -0.3% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Instrument Systems Design Complete<br>Linac Beam Available to Ring | Ring Beam Available to Target<br>Approve Critical Decision 4 – Start of Operations | N/A |
| Linac Coherent Light Source (SLAC) | | | |
| Cost Variance | 0% | | |
| Schedule Variance | -3.9% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 2b – Performance Baseline<br>Approve Critical Decision 3a – Start Long-Lead Procurement | Approve Critical Decision 3b – Start Construction | None |
| Center for Nanophase Materials Sciences (ORNL) | | | |
| Cost Variance | +0.1% | | |
| Schedule Variance | -0.6% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 4a – Start Initial Operations | Approve Critical Decision 4b – Start Full Operations | N/A |
| Center for Integrated Nanotechnologies (SNL/LANL) | | | |
| Cost Variance | -1.2% | | |
| Schedule Variance | -0.3% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | None | Approve Critical Decision 4a – Start Initial Operations | Approve Critical Decision 4b – Start of Full Operations |
| The Molecular Foundry (LBNL) | | | |
| Cost Variance | 0% | | |
| Schedule Variance | +3.9% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | None | Approve Critical Decision 4a – Start of Initial Operations | Approve Critical Decision 4b – Start of Full Operations |
| Center for Nanoscale Materials (ANL) | | | |
| Cost Variance | +1.2% | | |
| Schedule Variance | -2.6% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | None | Approve Critical Decision 4a – Start of Initial Operations | Approve Critical Decision 4b – Start of Full Operations |

| | FY 2005 Actual | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| Center for Functional Nanomaterials (BNL) | | | |
| Cost Variance | 0% | | |
| Schedule Variance | -26.3%[a] | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 3 – Start Construction | None | Approve Critical Decision 4a – Approve Building Occupancy |
| Instrumentation for Spallation Neutron Source I (ORNL) | | | |
| Cost Variance | -3.1% | | |
| Schedule Variance | -5.1% | | |
| Major (Levels 0 and 1) Milestones Completed or Committed to | Approve Critical Decision 2 for Instruments #1-3 – Performance Baseline<br>Approve Critical Decision 3 for Instruments #1-2 – Start Construction | Approve Critical Decision 2 for Instruments #4-5 – Performance Baseline<br>Approve Critical Decision 3 for Instruments #3 – Start Construction | Approve Critical Decision 3 for Instruments #4-5 – Start Construction |

## Construction and Infrastructure

### Linac Coherent Light Source (LCLS) Project

Most x-ray experiments performed at synchrotron radiation light sources produce static pictures of materials averaged over relatively long times. However, the electrons and atoms in molecules, crystal lattices, polymers, biomaterials, and all other materials are in constant motion. Merely measuring atomic "form" will not tell us all there is to know about molecular "function." We need to perform experiments that provide us with information on the motions of atoms in materials as well as their equilibrium positions. This will give us insight as never before possible into catalysis, chemical processes, protein folding, and molecular assembly.

The purpose of the LCLS Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source and that has pulse lengths measured in femtoseconds—the timescale of electronic and atomic motions. The advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons have revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be even more dramatic.

The LCLS Project will provide the world's first demonstration of an x-ray free-electron-laser (FEL) in the 1.5–15 Å (Angstrom) range. The characteristics of the light from the LCLS will open new realms of scientific inquiry and applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state

[a] The significant negative schedule variance for the CFN project is due to the DOE Acquisition Executive's decision to postpone CD-3 approval while BNL extended the procurement process for conventional facilities (CF) to secure a reasonably priced bid. CD-3 was ultimately approved and the CF contract was awarded in late FY 2005. Schedule recovery measures are in place that will ensure that CFN will be completed on time.

physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to create plasmas.

The LCLS project leverages capital investments in the existing SLAC linac as well as technologies developed for linear colliders and for the production of intense electron beams with radio-frequency photocathode guns. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through a newly constructed long undulator, the electron bunches will lead to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. Optical devices beyond the undulator manipulate the direction, size, energy, and duration of the x-ray beam and carry it to whatever experiment is under way. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation.

FY 2007 budget authority of $105,740,000 is requested. The estimated Total Project Cost is $379,000,000. Additional information on the LCLS Project is provided in the LCLS construction project data sheet, project number 05-R-320.

National Synchrotron Light Source – II (NSLS-II) Project

The NSLS-II, which is under development, will be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of one nanometer (nm), an energy resolution of 0.1 millielectron volt (meV), and the ultra-high sensitivity required to perform spectroscopy on a single atom.

NSLS-II will be the best storage-ring-based synchrotron light source in the world, but, more importantly, NSLS-II will be transformational in that it will open new regimes of scientific discovery and investigation. The ability to probe materials with 1 nm or better spatial resolution and to analyze their dynamics with 0.1 meV energy resolution will be truly revolutionary. For example, it will be possible to investigate the atomic and electronic structure and chemical composition of nanometer-scale objects under realistic in-situ device operating conditions. And it will be possible to investigate processes that change the energy or spin state of electrons, such as their interaction with the atomic lattice or other electrons or spins. These processes form the foundation of many diverse phenomena, such as photosynthesis and spin-based quantum computing, and the ability to study them with high spatial resolution will be unprecedented.

In FY 2007, budget authority is requested to begin Project Engineering and Design and for research and development (R&D) activities to address technical risks in four key areas—energy resolution, spatial resolution, superconducting undulators, and superconducting storage ring magnets. These R&D activities will be carried out at Brookhaven National Laboratory and by researchers elsewhere as needed. Additional information on the NSLS-II Project is provided in the NSLS Project Engineering Design data sheet, project number 07-SC-06.

Advanced Light Source (ALS) User Support Building Project

The ALS User Support Building to be located at the Lawerence Berkeley National Laboratory will provide high-quality user support space in sufficient quantity to accommodate the very rapid growth in the number of ALS users and to accommodate projected future expansion. Efficient use of the experimental beamlines at the ALS requires adjacent space for setting up experimental apparatus before quickly moving the apparatus into place. By the end of FY 2005, almost 40 beamlines were in simultaneous and nearly continuous operation for the use of 2,000 scientists and students. All available floor space for staging experiments is now occupied with operating beamlines, necessitating shutdown of beamlines and work stoppage when the experimental apparatus is built, when it is commissioned, and when it is moved into place at the beamline. Such use of beam time is unacceptable for advanced, state-of-the art instrumentation. In addition to being too small, the current user support space does not meet seismic building codes. Structural upgrades have been evaluated and would not be cost effective.The User Support Building will provide staging areas for ALS experiments, space for a long beamline that will extend from the floor of the ALS into the User Support Building, and temporary office space for visiting users. Additional information on the ALS User Support Building Project is provided in the User Support Building Project Engineering Design data sheet, project number 07-SC-12.

**General Plant Projects (GPP) and General Purpose Equipment (GPE)**

BES provides funding for GPP and GPE for Argonne National Laboratory, Ames Laboratory, and Oak Ridge National Laboratory.

**Workforce Development**

The BES program supports development of the R&D workforce through support of undergraduate researchers, graduate students working toward a doctoral degree, and postdoctoral associates developing their research and management skills. The R&D workforce developed under this program provides new scientific talent in areas of fundamental research and also provides talent for a wide variety of technical and industrial areas that require the problem solving abilities, computing skills, and technical skills developed through an education and experience in fundamental research. In addition, the BES scientific user facilities provide outstanding hands-on research experience to many young scientists. Thousands of students and post-doctoral investigators are among the researchers who conduct experiments at BES-supported facilities each year. The work that these young investigators perform at BES facilities is supported by a wide variety of sponsors including BES, other Departmental research programs, other federal agencies, and private institutions.

| | FY 2005 | FY 2006 estimate | FY 2007 estimate |
|---|---|---|---|
| # University Grants | 910 | 810 | 1,000 |
| Average Size | $150,000 | $150,000 | $150,000 |
| # Permanent Ph.D.s (FTEs) | 4,240 | 3,900 | 4,830 |
| # Postdoctoral Associates (FTEs) | 1,220 | 1,140 | 1,380 |
| # Graduate Students (FTEs) | 1,960 | 1,810 | 2,170 |

**External Independent Reviews**

Beginning in FY 2005, the costs of conducting External Independent Reviews (EIRs) for Capital Asset Projects greater than $5,000,000 within SC have been funded by SC. Examples of EIRs include conducting Performance Baseline EIRs prior to Critical Decision-2 (CD-2) to verify the accuracy of cost and schedule baseline estimates and conducting Construction/Execution Readiness EIRs, which are done for all Major System projects prior to CD-3. These funds, which are managed by the Office of Engineering and Construction Management, are exclusively used for EIRs directly related to these projects funded within SC. Beginning in FY 2007, the EIR business line will be financed via the Working Capital Fund to achieve parity on how EIRs are funded and to standardize the administration of these critical activities.

## Materials Sciences and Engineering

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Materials Sciences and Engineering | | | |
| Materials Sciences and Engineering Research | 290,400 | 274,220 | 335,099 |
| Facilities Operations | 330,826 | 444,675 | 644,885 |
| SBIR/STTR | — | 18,820 | 24,228 |
| Total, Materials Sciences and Engineering | 621,226 | 737,715 | 1,004,212 |

### Description

This subprogram extends the frontiers of materials sciences and engineering to expand the scientific foundations for the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use. The subprogram also plans, constructs, and operates the major x-ray scattering and neutron scattering scientific user facilities and the Nanoscale Science Research Centers.

Included within the $338,099,000 research component of this subprogram for FY 2007 are facility related activities such as R&D for new and upgraded facilities, accelerator and detector research, and all BES FY 2007 Major Items of Equipment. These activities total $50,453,000.

### Benefits

Ultimately the research leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use. For example, the fuel economy in automobiles is directly proportional to the weight of the automobile, and fundamental research on strength of materials has led to stronger, lighter materials, which directly affects fuel economy. The efficiency of a combustion engine is limited by the temperature and strength of materials, and fundamental research on alloys and ceramics has led to the development of materials that retain their strength at high temperatures. Research in semiconductor physics has led to substantial increases in the efficiency of photovoltaic materials for solar energy conversion. Fundamental research in condensed matter physics and ceramics has underpinned the development of practical high-temperature superconducting wires for more efficient transmission of electric power.

### Supporting Information

The subprogram supports basic research to understand the atomistic basis of materials properties and behavior and how to make materials perform better at acceptable cost through new methods of synthesis and processing. Basic research is supported in magnetic materials, semiconductors, superconductors, metals, ceramics, alloys, polymers, metallic glasses, ceramic matrix composites, catalytic materials, surface science, corrosion, neutron and x-ray scattering, chemical and physical properties, welding and joining, non-destructive evaluation, electron beam micro characterization, nanotechnology and microsystems, fluid dynamics and heat transfer in materials, nonlinear systems, and new instrumentation.

This subprogram, a premier sponsor of condensed matter and materials physics in the U.S., is the primary supporter of the BES user facilities including new facilities under construction: the Spallation

Neutron Source, the Nanoscale Science Research Centers, the Linac Coherent Light Source, the National Synchrotron Light Source-II, the User Support Building at LBNL, and a number of facility-related Major Items of Equipment.

**Selected FY 2005 Research Accomplishments**

- Synchrotron X-Rays Demonstrate Nanoscale Ferroelectricity. Films only a few atoms thick have been made that retain the controllable electric polarization needed for next generation nanoscale devices. Such ultrathin ferroelectric films have the potential to revolutionize future electronics, sensors, and actuators. Previous studies suggested that, as devices are miniaturized, they lose their ferroelectric character. These studies showed that ferroelectricity persists in films only 6 atoms thick. This landmark success was achieved using a unique instrument to observe thin film growth with high intensity x-rays from the Advanced Photon Source. X-rays reveal in real time the film structure as it grows, atomic layer by atomic layer. The in-situ x-ray techniques developed for this study can now be used to understand the synthesis and environmental interactions of other complex materials, thus addressing a wide range of energy-related challenges.
- A Superconductor that Tolerates Magnetic Fields. One of the biggest obstacles to the practical use of superconductors is the motion of magnetic flux due to an electric current in a superconductor. This motion of magnetic flux reduced the superconducting properties. A large research effort has gone into finding ways to prevent energy loss occurring from the movement of magnetic flux in copper oxide high temperature superconductors. It has been found that the magnetic flux in certain magnesium diboride films is intrinsically motionless, or "frozen," in applied magnetic fields up to 14 Tesla. Such a complete apathy to an applied magnetic field has never been seen before in any other superconductor. While the theoretical explanation for this behavior has eluded scientists, the experimental finding has drawn a lot of attention. This behavior may make it possible to fabricate superconducting wire that can carry very large electric currents.
- Using Electron Spin, not Electron Charge, to Carry Information. Today's computers are based on resistive circuitry using the movement of charged electrons. The resistance generates heat, and the removal of this heat is a fundamental limiting factor in creating the next generation of ultra small and ultra fast circuit elements. In a remarkable discovery, theorists have determined that in certain materials a spin current can be created with the application of a suitably oriented electric field, with no dissipation of energy. The spin current could potentially be used to carry out the same logic operations with no energy loss. This has been verified recently with experiments on gallium arsenide. This discovery may lead to computers with much greater capabilities including speed and capacity due to smaller circuit elements and with a significant reduction in energy loss.
- Plutonium Helps Understand Superconductivity's Mysteries. Magnetic resonance studies of the fundamental mechanism responsible for superconductivity in $PuCoGa_5$ reveal strong similarities to the high-$T_c$ copper oxide materials. These results confirm earlier theories that this unique family of plutonium superconductors is nearly magnetic. This is a new class of superconducting materials and forms a conceptual bridge between two families of magnetically mediated superconductors, the heavy fermion metals and the copper oxides. The discovery of additional classes of superconducting materials enhances our ability to understand the mechanisms responsible for high temperature superconductivity.
- Ultrafast Studies of Nanocrystals. The fastest phase transition between nanocrystal structures ever recorded has been observed by ultrafast laser techniques. The reversible structural change in nanocrystals of vanadium dioxide switches the material from a semiconductor to a metallic phase,

increasing the electrical conductivity by a factor of 100-10,000 depending on nanoparticle size. Correspondingly large changes from optical transparency to high reflectivity occur at the same time. Lasers with pulses as short as one ten-trillionth of a second were used to track the phase change in vanadium dioxide nanoparticles. This discovery may be key to possible applications requiring extremely rapid switching from transparent to reflective states. These include protective overlayers for sensitive infrared detectors, nonlinear optical switches, fiber-optic pressure sensors, and electrically or optically triggered transistors that could switch hundreds of times faster than conventional silicon devices.

- First Direct Observations of Quasiparticles. Quasiparticles provide a convenient simplification to describe the behavior of electrons in a superconductor. A quasiparticle can be thought of as a single particle moving through a system, surrounded by a cloud of other particles either pushed away or dragged along by its motion. Prior investigations of their dynamics have been indirect. Through the use of a new optical technique it was possible to perform the first direct study of the dynamics of quasiparticles in a superconductor. It was discovered that the quasiparticles can propagate remarkably far, several hundreds of nanometers. Knowledge of the dynamics of quasiparticles, specifically their rates of diffusion, scattering, trapping, and recombination, is critical for the both the applications and fundamental understanding of superconductivity.
- Confining Electrons in New Two-dimensional Materials. Transition metal oxides, like semiconductors, are materials that confine electrons to a plane. It may now be possible to construct near-perfect layered materials of two perovskite structured materials. It has been shown through computational models that a single layer of $LaTiO_3$ in $SrTiO_3$ will serve as an electron donor and positive charge layer to retain those electrons in a thin layer as a two-dimensional electron gas (2DEG). Electrons behaving like a 2DEG appear to be an exotic phenomenon, but they are not. Many semiconductor electronic devices operate by creating just such a gas by an applied electric field inducing a thin conducting region at an interface—the field effect transistor being the prime example. Such thin electron layers have become a valuable tool for scientists studying the ways in which electrons organize their collective behavior. By expanding the materials available to create 2DEGs, new, more diverse opportunities have been created to expand our knowledge of electronic behavior that in turn can produce new applications.
- Inexpensive Route to Solar Cells Using Nanomaterials. New and novel semiconductor nanocrystal-polymer solar cells with surprisingly high efficiencies have been fabricated. In a solar cell, the conversion of light energy to electrical current occurs at the nanometer scale. Thus the development of methods for controlling materials on this scale creates new opportunities for more advanced solar cells. These advances are required because, although solar cells based on silicon and gallium arsenide have achieved high efficiencies and have found a variety of markets, more widespread applications remain limited by their high cost of production. These new cells are formed in an inherently inexpensive process from a colloidal solution of semiconductor nanocrystals in a semiconducting polymer. The unique features of nanosized objects are exploited to optimize the cell performance by controlling the shape of the nanocrystals. The performance of the new cells already rivals that of the best polymer-based devices. While the power conversion efficiency is still below that of current amorphous silicon and single crystal devices, there are opportunities to increase performance further by adding additional nanocrystal components to capture more of the solar spectrum. Furthermore, the same methods can be extended to address other optoelectronic applications, such as photodetectors and light emitting diodes.

- Predicting Magnetism in Nanomaterials. As recording media and sensors become smaller and ever-denser, it is increasingly important to control magnetism in nanostructures. But the physical properties of magnetic nanostructures are linked in complex ways and are difficult to predict, much less control. In this work, the magnetic properties of a cobalt nano-wire next to a platinum surface step were predicted from first-principles. The results are in perfect agreement with experiment and show the importance of a proper quantum mechanical description of the interplay of different magnetic phenomena. This work, based on newly developed quantum mechanical models implemented on high-performance computers, shows that accurate predictions can be made for a nanostructure comprised of a few hundred atoms. With continued theoretical development and more powerful computers, this paves the way toward prediction and control of more complex and useful magnetic structures.
- Explaining Materials Deformation Mechanisms from Atomic-scale Measurements. Using the world's most advanced electron microscope, the first direct observations of atomic details in complex crystalline dislocation cores revealed the atomic mechanisms underlying the deformation of intermetallic compounds with complex crystal structures. It was discovered that the diffusion of chromium atoms into and out of the crystal dislocation cores hinders dislocation motion in Laves-phase $Cr_2Hf$, a model intermetallic compound, thus providing a clue as to the origin of the brittleness and poor low temperature ductility of these intermetallic alloys. The poor low-temperature ductility of these intermetallic alloys has prevented their fabrication and use for decades. Some of the most attractive high-strength alloys for advanced high-temperature fission and fossil energy conversion applications possess similar complicated atomic configurations and lack the low-temperature ductility required for their fabricated by conventional cold deformation processes without crack formation. This discovery provides new atomistic insight into the behavior of crystal dislocations in complex intermetallic compounds necessary to design new fabricable alloys with the required strength at high service temperatures.
- Discovery of Mechanism of Surface Mass Transport. Researchers have discovered that trace concentrations of sulfur can enhance the rate of mass transport on copper surfaces by many orders of magnitude and have established the atomic scale mechanism by which this enhancement occurs. This discovery was enabled by low-energy electron microscopy measurements of the motion of singe-atom-high steps on copper exposed to calibrated doses of sulfur. By comparing observations of the motion of these steps with theoretical predictions based on calculations of the electronic structure of the surface, this research established that surface mass transport is catalyzed by the formation of a large number of mobile copper sulfide clusters. Such highly mobile clusters are believed to be a common feature of impure surfaces. The enhanced mass transport allows the formation of much flatter and more defect free surfaces. This discovery provides insight to many previous puzzling observations of anomalous surface mass transport. It is an important advance towards the capability to control the nanoscale morphology of surfaces, a critical necessity for nanoscale applications.
- Superior Iron-based Alloys and Steels. Fundamental laws of alloying coupled with advanced microanalytical characterization led to the discovery that yttrium containing iron-based alloys substantially enhance the stability of the amorphous (non-crystalline) state. Two technical implications are: (1) large bulk physical dimensions of this class of amorphous alloys can be made and (2) this understanding provides a new direction for designing bulk amorphous metals for structural and functional applications. Bulk tool steel was fabricated that was twice as hard as conventional tool steel. These achievements are milestones in the science of amorphous metals and

the design of functional complex metallic alloys. Even more important, this research has demonstrated that microalloying is a new approach for designing bulk amorphous alloys. Their unique atomic configurations and the absence of a crystalline lattice allow bulk amorphous metals to outperform their crystalline counterparts by exhibiting superior magnetic and mechanical properties and corrosion resistance coupled with high thermal stability.

- Fracture Resistance Mechanism in Ceramics. Structural ceramics are complex structures of micron-sized matrix grains separated by a nanoscale intergranular film. For many years it has been observed that certain additives, specifically rare-earth atoms, influence the ceramic's fracture resistance. But detailed information about how this effect is achieved and how it can be controlled had been inaccessible with current diagnostic capabilities. Now, new scanning transmission electron microscopy (STEM) and associated chemical analysis techniques have revealed the local atomic structure and bonding characteristics of the grain boundaries with close to atomic resolution. Applied to silicon nitride ceramics containing a range of rare-earth additives, these methods together have revealed how each atom bonds at a specific location depending on atom radius, electronic configuration and the presence of oxygen; this variation in bonding sites can be directly related to the fracture resistance or toughness of the ceramic.
- Better Protective Coatings. Previously unattainable insight into stress development and failure mechanisms in thermally grown surface oxides on metal alloys has been obtained by a new in-situ synchrotron x-ray technique. This technique enabled, for the first time, the uncoupling and isolation of mechanical stress contributions from oxide growth, phase transformations, and creep deformation processes. For pure thermally-grown alumina, steady state oxidation creates compressive stresses. However, when certain "reactive elements" are added to the alloy, it is found that tensile stresses develop instead. Maximizing the tensile offset can lead to dramatic improvement in performance of a protective oxide. A 10 percent shift in the tensile direction can translate to a 40 percent improvement in operating lifetime. Better control of early stage oxidation leads to thinner, and thus longer lifetime protective oxides by speeding the transformation to a stable oxide structure. These results underpin future alloy development for high-temperature nuclear and fossil energy generation technologies and more fuel efficient jet engine applications where operating lifetime has great economic value.
- New Composite Materials that Respond to Magnetic Fields. Magnetic-field-structured composites are a novel class of material in which magnetic particles, dispersed in a polymerizable medium, are organized into chains and other structures by magnetic fields while the polymer solidifies. These chains of particles can be electrically conductive, and this electrical conductivity can be extremely sensitive to temperature, pressure, and chemical vapors that penetrate and swell the polymer. In the present work it was demonstrated that even modest magnetic fields produced by simple copper coils cause these materials to contract significantly, like artificial muscles. This contraction was found to be accompanied by an enormous, 50,000-fold increase in electrical conductivity. This is by far the largest "magnetoresistance" effect ever observed in such modest magnetic fields and paves the way to using magnetic fields to control heat and current transport in micro and nano machines, and to tailoring the sensing response of these materials.
- The "Giant Proximity Effect." The reproducible confirmation of the existence of a Giant Proximity Effect (GPE) has challenged experimentalists for over a decade. In the traditional Proximity Effect (PE), a very thin layer of normal metal, when placed between two thicker superconductor slices, behaves like a superconductor. That is, superconducting or paired electrons retain phase coherence even while separated by the normal metal gap. In the newly discovered GPE, the normal-metal barrier layer is as much as 100 times thicker than in the PE case, a result that stands outside of any

present theories. In addition to challenging the theoretical community and providing new clues to the causes of high-temperature superconductivity, this result may lead to new advances in superconducting circuitry as it is relatively easy to prepare reproducible thick barriers which will improve device uniformity and yield.

- World's Smallest Nanomotor. The smallest synthetic motor—a 300 nanometer gold rotor on a carbon nanotube shaft—has been demonstrated. This "nanomotor" continues the dramatic advances in the miniaturization of electromechanical devices and is a key step in the realization of practical synthetic nanometer-scale electromechanical systems (NEMS). In initial testing, the rotor rotated on its nanotube shaft for thousands of cycles with no apparent wear or degradation in performance. This is attributed to the unique low-friction characteristics of the carbon nanotube shaft. The new motor design has significant potential for NEMS applications. It should be possible to fabricate arrays of orientationally-ordered nanotube-based actuators on substrates by using alignment techniques.
- Magnetohydrodynamic Turbulence in Liquid Metals. Application of a strong magnetic field can completely change flow characteristics of an electrically conducting fluid. The transformation may occur in processes ranging from the generation of sunspots to crystal growth. One particular aspect of this phenomenon, the damping of flow variations along the magnetic field lines and the corresponding development of elongated or even two-dimensional flow structures, affect nearly all aspects of turbulent flow behavior, including heat transfer and mixing. In a series of high resolution numerical experiments it has been shown that the anisotropy of flow (or directionality of flow) patterns is a robust universal feature determined primarily by the strength of the magnetic field, conductivity, and kinetic energy. Furthermore, the elongation of flow patterns is approximately the same for flow structures of different size. This property can be effectively employed for accurate modeling of magnetohydrodynamic turbulence. The results of the work are relevant to technological applications, such as continuous casting of steel, crystal growth, and development of lithium breeding blankets for fusion reactors.
- Nanoparticle Catalysts. Methods were developed for depositing and stabilizing nanometer-sized platinum group metals, including palladium and rhodium, on surfaces of carbon nanotubes in supercritical fluid carbon dioxide. Uniformly distributed monometallic and bimetallic nanoparticles with narrow size distributions are formed on the surfaces of the carbon nanotubes. The carbon nanotube-supported palladium and rhodium nanoparticles demonstrated improved performance over commercial carbon-based palladium and rhodium catalysts for hydrogenation of olefins and aromatic compounds. These new nanoscale catalysts are currently being tested as electrocatalysts for low temperature polymer electrode fuel cells applications.

**Selected FY 2005 Facility Accomplishments**

- The Advanced Light Source (ALS)
  - Beam-Size Stability Improved. Over the last five years, elliptically polarizing undulators (EPUs) have been used very successfully at the ALS to generate high-intensity photon beams with variable photon polarization (from linear to circular). However, users were not completely satisfied with the EPUs performance because they degraded the beam quality by increasing the photon beam size. Based on detailed magnet measurements, a system was developed that maintains a constant beam size. It is now being employed in routine user operation solving a problem that has affected many other light sources.

- New Undulator Beamline for High-Resolution Photoemission Electron Microscopy. Beamline 11.0.1 is a new elliptically polarizing undulator (EPU) beamline dedicated to photoemission electron microscopy (PEEM) at the ALS. An EPU, the third installed at the ALS, delivers light into the new beamline, which began commissioning March 2005. With full polarization control and continuous coverage optimized over key energy regions, this beamline will be an attractive user facility for organic and magnetic polarization-contrast microscopy. This beamline will have an aberration-corrected photoemission electron microscope (PEEM-3) with a spatial resolution of approximately 5 nanometers.

- New In-Vacuum Undulator Beamline for Femtosecond X-ray Studies. Beamline 6.0.1 for soft x-ray science with ultrashort photon pulses of 200 femtoseconds was ready for commissioning in July 2005. The beamline is unique in the U.S. and will be made available to users in FY 2006. The primary components are a vacuum undulator to produce x-rays over a wide photon-energy range, optical components, including a spectrograph for recording an entire x-ray absorption spectrum from one photon pulse, and a high-repetition-rate femtosecond laser system.

▪ The Advanced Photon Source (APS)

- More Stable Beams. Using a technique pioneered at the APS, 175 girders supporting accelerator components in the APS storage ring have been displaced by as much as 6 mm during scheduled tri-annual maintenance periods over the last seven years, eliminating the stray radiation background signals. As a result, photon beam position monitors (BPMs) for insertion devices over the entire storage ring circumference are now operating on line. The APS leads the world in the use of photon BPMs for insertion device beamlines. Use of these monitors has improved long-term x-ray beam angular stability by more than a factor of five. Users are able to scan the x-ray photon energy by changing the insertion device gap on demand, while still maintaining superior photon beam stability on their samples. The payoff is improved ability to resolve micron and nanometer-sized features in samples

- Improved Timing Experiments. The x-ray pulse structure at the APS is on the order of 100 picoseconds. This pulse width enables special classes of timing experiments where the physical phenomena require fast time resolution. Recent experiments at the APS using this technique have involved the study of porphyrins that may one day form the building blocks of novel catalysts, photonic devices, and efficient solar-power units. The APS has a special operating mode to facilitate these types of measurements. In this mode, a single x-ray timing pulse is isolated from the other x-ray pulses. The intensity in the pulse is determined by the amount of charge stored in the isolated electron bunch that generates the photon pulse. Recent changes to the storage ring top-up injection method, which allows the APS linear accelerator to vary the injection charge along with increasing the injection frequency from two minutes to one minute, have resulted in doubling the single pulse-intensity without adversely affecting the non-timing experiments.

- Improved Mirrors for X-ray Focusing. Elliptically-shaped mirrors based on new technology developed at the Advanced Photon Source are being used to achieve unprecedented focusing of high-brightness x-ray beams. These mirrors are especially useful for producing the microbeams that are used to probe the composition and structure of materials. They are being applied to studies such as microstructural analyses of structural changes arising from welding operations and detailed investigations of the three-dimensional structure of complex crystalline samples.

- Nanoprobe Beamline Commissioned for First Experiments. The world's first hard x-ray nanoprobe was activated in March 2005, at the APS. The Nanoprobe beamline is a central component of the new Center for Nanoscale Materials at Argonne National Laboratory. The x-ray nanoprobe will have a spatial resolution of 30 nanometers or better, the highest of any hard x-ray microscopy beamline in the world. It will offer fluorescence, diffraction, and transmission imaging in the x-ray spectral range of 3-30 keV, making it a valuable tool for studying nanomaterials.

- The National Synchrotron Light Source (NSLS)
  - New X-ray Micro-Diffraction Instrument. This instrument to be used for nanoscale research was developed at the X13B beamline to take advantage of the small source size of the in-vacuum mini-gap undulator in the X13 straight section of the NSLS x-ray ring. It consists of five main subsystems: monochromator, focusing optics, sample manipulator, charge-coupled detector (CCD) area detector, and a point detector with two degrees of freedom. The sample stages are equipped with integrated submicron position encoders for excellent positional precision and repeatability. The point detector assembly allows the use of analyzer crystals to obtain better resolution. A key design feature is the close attention paid to mechanical coupling of the focusing optics to the sample positioner to reduce vibrations and improve the microscope stability for the users.
  - Elliptically-Polarized Wiggler Beamline Upgrade. The Elliptically-Polarized Wiggler (EPW) located in the X13 straight section of the NSLS x-ray is a unique radiation source that produces time-varying elliptically-polarized x-rays for magnetism studies. A major upgrade was performed on beamline X13A to enhance its performance. It included replacement of the existing horizontal focusing mirror, which had been plagued by poor reflectivity as well as mechanical and thermal stability problems, with a new water-cooled spherical mirror. The new mirror system increases the horizontal photon collecting angle by a factor of two and is fully motorized to allow precise manipulation and optimization of the mirror's position. In addition, the beamline interlock and control systems were upgraded. The beamline upgrade has resulted in an order of magnitude increase in the photon intensity delivered to the sample, and the elimination of mechanical and thermal instabilities. These improvements have led to more efficient use of the beamline and increased magnetic sensitivity in the measurements.
  - Development of a Photon-Counting Silicon Microstrip Array Detector. The NSLS detector group has developed an extremely versatile 1-dimensional position sensitive detector. It is based on custom microelectronics developed at Brookhaven National Laboratory, and consists of a linear array of silicon photodiodes, each 0.125 x 4 mm, which is connected to a set of 32-channel custom integrated circuits and a microprocessor system. The detector system's performance is several orders of magnitude better than one can achieve with charge-coupled type detectors. It is easily adaptable to as large an array as is needed by the application. For example, arrays of 320 and 640 strips, 40 and 80mm long have been fabricated for real-time x-ray scattering.
  - X-ray Ring Lattice Symmetry Restored. The most direct benefit for the NSLS user community was the restoration of the x-ray ring magnetic field lattice symmetry, which for many beamlines resulted in a 25 percent reduction of the horizontal beam size and an increase in photon intensity delivered to a sample. The desired eight fold symmetry of the x-ray ring magnet lattice can be lost from errors in the x-ray ring quadrupole field strengths. The quadrupole errors can be partially compensated by trim coils available in the x-ray ring for one of the quadrupole magnet families. These errors were determined from an elaborate analysis of the electron orbit measurements taken as quadrupole magnet field strengths were systematically varied. This

improvement allowed the NSLS to restore the eight fold symmetric x-ray ring magnet settings for routine operations.

- The Stanford Synchrotron Radiation Laboratory (SSRL)
  - First SPEAR3 Run Completed. In the commissioning run for the new SPEAR3 accelerator, the facility proved to be exceptionally reliable, providing very stable beam for a very high percent (97) of the scheduled time. This is higher than ever recorded with SPEAR2, and an exceptional achievement for a new storage ring. The user run commenced in March and the SPEAR3 storage ring operated at 3 GeV/100 mA and provided 30+ hour life times. (The average uptime over the past five years was 96%.) During the run, users on 239 different proposals received beam time in a total of 466 experimental starts involving 1,516 researchers.
  - First High-Current SPEAR3 Tests Performed. SSRL conducted three special 8-hour shifts of SPEAR3 operation with currents above the official safety envelope value of 100 mA. These high-current test shifts took place on swing shifts with the experimental floor cleared of non-radiation workers. The main purpose of these tests was to determine if multi-bunch electron beam instabilities will be encountered at higher current operation, in which case a program to implement a costly multi-bunch feedback system would have to be launched. Other potential problems, primarily excessive component heating, are also of concern. The current reached in these tests was limited to 225 mA by the power rating of some absorbers in a legacy insertion device chamber. This current was reached and a comprehensive search revealed no apparent beam instabilities.
  - New Methods Developed for Studying Structures of Nanomaterials. The reactivity and properties of nanomaterials are highly influenced by particle size and atomic-scale structure. Researchers at SSRL have recently demonstrated that the combined use of several x-ray scattering and absorption measurement techniques leads to quantum leaps in understanding the structures of nanomaterials. X-ray scattering measurements allow experimenters to combine size and shape information with structural information to remove the small-particle size contribution to x-ray diffraction peak broadening, whereas x-ray absorption measurements provide complementary, metal-specific information on local atomic structure in disordered materials. Measurements on zinc sulfide have conclusively demonstrated that structural relaxation of surface atoms causes inhomogeneous internal strain, markedly altering its material properties. This multi-technique nano-characterization approach has further been advanced by developing methods for the routine characterization of bacterial nano-minerals under fully-hydrated *in-situ* conditions. Bacterial nanominerals are an important class of naturally occurring nanomaterials that help to control the composition of the atmosphere, the potability of natural waters, and the arability of soils. This multiple-technique method provides unique information of wide interest to the nanoscience community.

- The Intense Pulsed Neutron Source (IPNS)
  - Simultaneous Measurement of Mixed-conductor Lattice Relaxation, Diffusion, and Gas Conversion. The General Purpose Powder Diffractometer (GPPD) at the IPNS is equipped with a specially designed controlled-atmosphere furnace, where samples in pellet or hollow-tube form are exposed to mixtures of gases to control oxygen and hydrogen content from highly oxidizing to highly reducing environments. Using two separate gas delivery "circuits," simulated membrane operation conditions can be achieved whereby the responses of oxygen-permeable membranes to strong oxygen partial pressure gradients can be studied. Exhaust gases are

analyzed with a Residual Gas Analyzer to probe for leakage and to quantify gas conversion reactions. Dense ceramic components with mixed-conduction properties and high oxygen permeability are important as membranes for oxygen separation and solid oxide fuel cell applications. Membranes are typically operated at elevated temperatures (800-1000°C) and exposed to large oxygen partial pressure gradients. This experiment reproduces the conditions under which these membranes will be used commercially and provides insights into the unusual differential oxygen partial pressure stability of these materials.

- Accelerator Systems Improvements. Efforts include: completion of the beamline-magnet power supply upgrades, replacing the originals with higher-efficiency and better regulated units; completion of a full year of operation of the first of two new kicker-magnet power supplies; and completion of full-power tests of the new third-rf system that will be installed in the synchrotron ring to provide new proton beam capture and handling capabilities.
- National Neutron and X-ray Scattering School. During August 2005, Argonne National Laboratory again hosted the National School on Neutron and X-Ray Scattering. The school continues to attract outstanding graduate students and post-doctoral appointees with 150 applications for the 60 positions available in 2005. The intensive training introduces students to the theory of, and provides hands-on experimentation in, x-ray and neutron scattering.

▪ The Manuel Lujan Jr. Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE)

- Neutron Scattering Winter Schools. The First and Second Annual LANSCE Neutron Scattering Winter Schools were held, with 30 students from a wide geographical distribution attending each School. The 2004 topic was magnetism and the 2005 topic was mechanical properties of materials. During nine intensive days in Los Alamos, students had lectures from world experts on the key materials issues for the School theme, modeling and theory, and neutron scattering techniques addressing these issues. In addition, the students had the opportunity to gain hands-on experience in neutron-scattering techniques and data analysis.
- New Sample Environments. A major emphasis on sample environments in FY 2005 has greatly enhanced the low temperature, high field, and high pressure possibilities for user experiments. Investments in new low temperature sample environments, high pressure instrumentation, sample goniometers, and support staff have made users more productive. Along with the 11-Tesla superconducting magnet commissioned in 2004, the Lujan Center's suite of sample environments for condensed matter physics has dramatically improved in FY 2005. A rheometer designed to synchronize with the 20 Hz Lujan Center pulsed neutron beam is expected to be tested in FY 2005. It will provide a unique capability to impose accurate hydrodynamic shear on polymer solutions and colloidal suspensions while performing structural measurements by small-angle neutron scattering.
- Instruments Enhancement. The High Intensity Powder Diffractometer (HIPD) and the Single Crystal Diffractometer (SCD) have received upgrades to software, shielding, alignments, and hardware that have increased their neutron intensity, user throughput, and efficiency. New hardware and software controls on the Low-Q Diffractometer (LQD) and a new detector have made small angle neutron scattering (SANS) more effective.

- The High Flux Isotope Reactor (HFIR)
  - Common Guide Casings for Seven New Instruments Installed. Neutron guides transport cold neutrons (energies ~0.1–20 meV) with little loss in flux. This permits one to transport neutron beams from the source to instruments several tens of meters away. This lowers the instrumental background noise from gamma rays and unwanted neutrons since one can place the instruments far from the source. Also, the guides have a slight curvature which removes the "line-of-sight" view of the neutron source and further reduces this background. The guides are made by coating glass with layered coatings called supermirrors which are highly reflective for neutrons. These flat, coated glass plates are then assembled to form hollow rectangular cross-sectioned pipes with the coated sides forming the interior walls of the pipes. These guides will be illuminated with neutrons produced by the new HFIR cold source to be installed early in 2006.
  - HB-4 Shield Tunnel and Velocity Selector Shielding Installed. A great deal of neutron shielding is required to shield the exit of the new HFIR cold source and components of the cold neutron beamlines. The first and largest general section of shielding for the new instruments was constructed. Also, the lead shielding for the velocity selectors for the two small angle neutron scattering (SANS) instruments was assembled. These components are essential for the new Center for Neutron Scattering cold neutron spectrometers.
  - SANS 1 Detector Tank and Internal Components Installed. The largest component for the first Small Angle Neutron Scattering (SANS) instruments has been installed. This giant tank will contain the detector for this instrument. The 1 meter square detector will ride on rails inside the evacuated volume of the tank.
  - The Neutron Reflectometer Commissioned. A new instrument, the neutron reflectometer, was commissioned for use in the general user program at the HFIR Center for Neutron Scattering. This machine is optimized for the studies of surfaces and interfaces. It is the fifth Cold Neutron Source instrument fully commissioned and will be used for the studies of polymers, biomaterials, thin solid films, and surfactants.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Materials Sciences and Engineering Research** .............................. | **290,400** | **274,220** | **335,009** |
| ▪ **Structure and Composition of Materials** ................................ | **24,907** | **16,943** | **22,245** |

This activity supports basic research on the structure and composition of materials including research on the arrangement and identity of atoms and molecules in materials, and the development of quantitative characterization techniques, theories, and models describing how atoms and molecules are arranged. Also sought are the mechanisms by which the arrangements are created and evolve. Increasingly important are the structure and composition of inhomogeneities including defects and the morphology of interfaces, surfaces, and precipitates.

The properties of materials used in all areas of energy technology depend upon their structure. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the structural characteristics of advanced

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| FY 2005 | FY 2006 | FY 2007 |

materials. This dependence occurs because the spatial and chemical inhomogeneities in materials (e.g., dislocations, grain boundaries, magnetic domain walls, and precipitates) determine and control critical behaviors such as fracture toughness, ease of fabrication by deformation processing, charge transport and storage capacity, surface/catalytic reactivity, superconducting parameters, magnetic behavior, corrosion susceptibility, etc.

Capital equipment is provided for items such as new electron microscopes and improvements to existing instruments.

In FY 2007, funding will continue on advanced instruments with capabilities to characterize and interpret atomic configurations and packing arrangements at the nanoscale with improved resolution and accuracy, including the ability to determine composition, bonding, and physical properties of materials. Within this funding, there are increases to support the development of advanced electron microscopy and scanning probe techniques ($+763,000), ultrafast electron scattering probes as companion tools to ultrafast photon probes ($+1,000,000), for mid-scale instrumentation to develop new experimental tools and techniques for atomic scale structural characterization ($+2,000,000), for research related to the hydrogen economy ($+100,000), and for solar energy conversion ($+1,439,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Mechanical Behavior and Radiation Effects** .......................... | **14,008** | **13,037** | **18,195** |

This activity supports basic research to understand the deformation, embrittlement, fracture, and radiation damage of materials. Concerns include the behavior of materials under repeated or cyclic stress, high rates of stress application as in impact loading, and over a range of temperatures corresponding to the stress and temperature conditions in present and anticipated future energy conversion systems. The objective is to achieve an atomic level understanding of the relationship between mechanical behavior and defects in materials, including defect formation, growth, migration, and propagation. This research aims to build on this atomic level understanding in order to develop predictive models for the design of materials having superior mechanical behavior, with some emphasis on very high temperatures. The focus of basic research in radiation effects is to achieve an atomic-level fundamental understanding of mechanisms of radiation damage and how to design radiation-tolerant materials. Concerns include radiation induced embrittlement and radiation assisted stress-corrosion cracking. Other issues include achieving an atomic level understanding of amorphization mechanisms (transition from crystalline to a non-crystalline phase) and the modification of surface behavior by techniques such as ion implantation.

This program contributes to DOE missions in the areas of fossil energy, fusion energy, nuclear energy, transportation systems, industrial technologies, defense programs, radioactive waste storage, energy efficiency, and environment management. This research helps understand load-bearing capability, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility or deformability of materials that is critical to their ease of fabrication, and radiation effects including understanding and modeling of radiation damage and surface modification using ion implantation. This activity relates to energy production and conversion through the need for failure resistant materials that perform reliably in the hostile and demanding environments of energy production and use. This program contributes to understanding

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|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

mechanical properties of materials and aspects of nuclear technologies ranging from radioactive waste storage to extending the lifetime of nuclear facilities.

Capital equipment is provided for items such as in-situ high-temperature furnaces, and characterization instrumentation.

In FY 2007, funding will continue support for research on understanding the mechanisms that are related to both the deformation and degradation of materials. Specific emphasis will be on nanoscale mechanics, and in particular the complex mechanical interactions of fundamental building blocks in directed self-assembly. The program also supports the development of new theoretical and experimental tools to probe the deformation and degradation behaviors at the nanoscale. Within this funding, there is an increase for ongoing materials research in support of materials related to advanced nuclear reactor fuel cycles ($+5,158,000).

| | FY 2005 | FY 2006 | FY 2007 |
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| ▪ **Physical Behavior of Materials** ................................................ | **25,551** | **24,677** | **29,756** |

This activity supports basic research at the atomic and molecular level to understand, predict, and control physical behavior and functional properties of materials by developing models for the response of materials to environmental stimuli such as: temperature, electromagnetic fields, chemical environments, and proximity of surfaces or interfaces. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the superconducting properties for high-temperature superconductors; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures encountered in energy conversion processes; and diffusion and transport of ions in ceramic electrolytes for improved performance in batteries and fuel cells.

Research underpins the missions of DOE by developing the basic science necessary for improving the reliability of materials in mechanical and electrical applications and for improving the generation and storage of energy. With increased demands being placed on materials in real-world environments (extreme temperatures, strong magnetic fields, hostile chemical environments, etc.), understanding how their behavior is linked to their surroundings and treatment history is critical.

Capital equipment is provided for items such as spectroscopic instruments, instruments for electronic and magnetic property measurement, and analytical instruments for chemical and electrochemical analysis.

In FY 2007, major activities will include basic research for solar to electricity conversion. Areas of emphasis include polycrystalline, nanocrystalline, and organic materials to replace expensive single crystals; innovative design of interpenetrating photoconversion materials networks to improve charge separation and collection efficiency; and the development of novel processes to obtain extremely high conversion efficiencies at modest cost. With the anticipated vigorous development of new types of nanoscale materials, new opportunities will emerge to dramatically improve solar energy conversion efficiency. Within this funding, there are increases to support solar conversion research ($+4,379,000) and research activities related to the hydrogen economy ($+700,000).

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| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Synthesis and Processing Science** ........................................... | **15,149** | **17,083** | **21,022** |

This activity supports basic research to understand and develop innovative ways to make materials with desired structure, properties, or behavior. Examples of activities in synthesis and processing include the growth of single crystals of controlled orientation, purity, and perfection; the formation of thin films of controlled structure and orientation by various techniques; atomic and molecular self assembly to create and explore new materials; nanostructured materials including those that mimic the structure of natural materials; the preparation and control of powder or particulate matter for consolidation into bulk form by many alternative processes; sol-gel processes; the welding and joining of materials including dissimilar materials or materials with substantial differences in their coefficients of thermal expansion; plasma, laser, and charged particle beam surface modification and materials synthesis; and myriad issues in process science. This activity also includes development of in-situ measurement techniques and capabilities to quantitatively determine variations in the energetics and kinetics of growth and formation processes on atomic or nanometer length scales.

This activity includes the operation of the Materials Preparation Center at the Ames Laboratory, which develops innovative and superior processes for materials preparation and provides small quantities of research-grade, controlled-purity materials and crystals that are not otherwise available to academic, governmental, and industrial research communities to be used for research purposes.

This activity underpins many of the DOE technology programs, and appropriate linkages have been established in the areas of light-weight, metallic alloys; structural ceramics; high-temperature superconductors; and industrial materials, such as intermetallic alloys.

Capital equipment includes controlled crystal growth apparatus, furnaces, lasers, chemical vapor and molecular beam epitaxial processing equipment, plasma and ion sources, and deposition equipment.

In FY 2007, funding will include continued support for research on nanoscale synthesis and processing. Major emphasis will be on providing synthesis and processing capabilities to enable the manipulation of individual spin, charge, and atomic configurations in ways to probe the atomistic basis of the emergent behavior. Research on emergent behavior will have a significant impact on developing new materials and devices for energy applications, including spin-based electronics and multifunctional sensors. Within this funding, there are increases to initiate new emergent behavior research ($+1,000,000), research activities related to hydrogen economy ($+1,500,000), and solar energy conversion ($+1,439,000).

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| ▪ **Engineering Research** ............................................................. | **5,306** | **2,444** | **1,000** |

This activity supports fundamental atomic or nanoscale studies of the conduction of heat in terms of the interactions of phonons (or crystal lattice vibrations) with crystalline defects and impurities and the transfer of mass and energy in turbulent flow in geometrically constrained systems and the mechanics of nanoscale systems.

The performance, safety, and economics of fission, fusion, fossil, and transportation energy conversion systems depend on a thorough understanding of heat transfer in regimes of complex, multi-phase fluid flow and the ability to provide reliable early warning of impending catastrophic fracture or other failure.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

In FY 2007, in order to emphasize other research activities described herein, selected activities in engineering research will be terminated, including nanoindentation, fluid behavior during solidification, heat transfer, and multiphase fluid flow.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Neutron and X-ray Scattering** ............................................... | **46,061** | **45,141** | **62,055** |

This activity supports basic research in condensed matter physics and materials physics using neutron and x-ray scattering capabilities, primarily at major BES-supported user facilities. Research seeks to achieve a fundamental understanding of the atomic, electronic, and magnetic structures of materials as well as the relationship of these structures and excitations to the physical properties of materials. The increasing complexity of such energy-relevant materials as nanoscale catalysts, superconductors, semiconductors, and magnets requires ever more sophisticated neutron and x-ray scattering techniques to extract useful knowledge and develop new theories for the behavior of these materials. Both ordered and disordered materials are of interest as are strongly correlated electron systems, surface and interface phenomena, and behavior under environmental variables such as temperature, pressure, and magnetic field. X-ray and neutron, together with the electron scattering probes supported under Structure and Composition of Materials and Electron-beam Microcharacterization Facilities, are the primary tools for characterizing the atomic, electronic, and magnetic structures of materials.

Research in the areas of nanostructured materials and novel hydrogen storage media will be continued using the structural and chemical information garnered from x-ray and especially neutron scattering. Structural studies on carbon-based hydrogen storage media-such as nanotubes, nanohorns, fullerenes, and nanoscale hydrides also will be performed to reveal the site of hydrogen incorporation and the mechanisms of hydrogen storage. The knowledge and technique developed in this activity have broad applicability in developing new materials for efficient and environmentally acceptable energy technologies.

Capital equipment is provided for items such as detectors, monochromators, mirrors, and beamline instrumentation at all of the facilities.

In FY 2007, activities will be initiated in ultrafast materials science research with an emphasis on understanding the physics of strongly correlated systems and systems at the nanoscale; properties and behavior of materials at high pressure magnetic fields; real-time, in-situ characterization of materials synthesis; exploratory research on next generation instrument concepts for synchrotron light sources and neutron sources; and studies of structure and dynamics in hydrogen storage materials ($+9,614,000). Additional funding is provided for the development of new research activities in photon-based ultrafast materials science ($+4,000,000), the development of mid-scale instrumentation including end stations at the synchrotron light sources and neutron scattering facilities ($+1,000,000), and research related to the hydrogen economy ($+2,300,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Experimental Condensed Matter Physics**............................... | **41,024** | **36,691** | **47,480** |

This activity supports condensed matter physics with emphases in electronic structure, surfaces, and interfaces and new materials. Research includes measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. This activity includes the design and synthesis of new materials with new and improved

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

properties. These materials include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The development of new techniques and instruments including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy is a major component of this activity. Measurements are made under extreme conditions of temperature, pressure, and magnetic field.

This research is aimed at a fundamental understanding of the behavior of materials that underpin DOE technologies. This activity supports research in photovoltaics, superconductivity, magnetic materials, thermoelectrics, and optical materials which underpin various technology programs in Energy Efficiency and Renewable Energy (EERE). Research in superconductivity and photovaltaics especially is coordinated with the Solar technologies program in EERE. In addition, this activity supports the strategically important information technology and electronics industries in the fields of semiconductor physics, electronics, and spintronics research. The petroleum recovery efforts of Fossil Energy (FE) and the clean-up efforts of Environmental Management (EM) programs are supported through research on granular materials and on fluids.

Capital equipment is provided for crystal growth equipment, scanning tunneling microscopes, electron detectors for photoemission experiments, sample chambers, superconducting magnets, and computers.

In FY 2007, major activities will continue in the development of nanomaterials for both energy conversion and hydrogen energy storage, which exhibit size-dependent properties that are not seen in macroscopic solid state materials. Enhanced electrical, thermal, mechanical, optical, and chemical properties have shown that these new nanomaterials could lead to dramatic improvements in the technologies relevant to fuel cells, batteries, capacitors, nanoelectronics, sensors, photovoltaics, thermal management, super-strong lightweight materials, hydrogen storage, and electrical power transmission. Within this funding, there is an increase to initiate mid-scale instrumentation for the synthesis of new materials and the growth of high quality single crystals ($+2,500,000) and for solar energy conversion ($+4,939,000). Additional funding is provided for research related to the hydrogen economy ($+3,350,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Condensed Matter Theory** ........................................................ | **19,798** | **22,888** | **27,408** |

This activity supports basic research in theory, modeling, and simulations of the condensed matters, and it complements the Experimental Condensed Matter Physics activity. A current major thrust is in nanoscale science where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are not well understood. For the simplest semiconductor systems, carbon nanotubes, and similar “elementary” systems, there has been considerable progress. However, progress in establishing the theoretical framework for more complex materials and hybrid structures has been limited. Computer simulations will play a major role in understanding materials at the nanometer scale and in the development “by design” of new nanoscale materials and devices. The greatest challenges and opportunities are in the transition regions where nanoscale phenomena are just beginning to emerge from the macroscopic and microscale regimes.

The Computational Materials Sciences Network supports cooperative research teams for studies requiring numerous researchers with diverse expertise. Examples include fracture mechanics—

understanding ductile and brittle behavior; microstructural evolution in which microstructural effects on the mechanics of materials; magnetic materials across all length scales; excited state electronic structure and response functions; and strongly correlated electron systems. The knowledge and computational tools developed in this activity have broad applicability on programs supported by Energy Efficiency and Renewable Energy and National Nuclear Security Administration.

Capital equipment will be provided for items such as computer workstations, beamline instruments, ion implantation, and analytical instruments.

In FY 2007, major activities will include both theoretical and computational approaches capable of interrogating systems to gain direct insight on the mechanisms underpinning the cooperative behavior of complex systems. Unlocking the mysteries of these systems will lay the scientific foundation for designing and engineering new multifunctional materials, devices and sensors with exquisitely sensitive properties. Within this funding, there are increases to support new emergent behavior research ($+1,500,000), research related to hydrogen production, storage, and use ($+1,100,000), and for solar energy conversion ($+1,920,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Materials Chemistry** ......... | **46,860** | **40,694** | **49,748** |

This activity supports basic research on the design, synthesis, characterization, and properties of novel materials and structures. The portfolio emphasizes solid-state chemistry, surface chemistry, and interfacial chemistry. It includes investigation of novel materials such as low-dimensional solids, self-assembled monolayers, electrocatalysts, cluster and nanocrystal-based materials, conducting and electroluminescent polymers, organic superconductors and magnets, complex fluids, hybrid materials, biomolecular materials and solid-state neutron detectors. There is a continued interest in the synthesis of new complex materials with nanoscale structural control and unique material properties that originate at the nanoscale. Significant research opportunities also exist at the biology/materials science interface. A wide variety of experimental techniques are employed to characterize these materials including x-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and x-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as surface force apparatus in combination with various spectroscopies.

The research in this activity underpins many energy-related technological areas such as batteries and fuel cells, catalysis, friction and lubrication, membranes, sensors and electronics, and materials aspects of environmental chemistry. The development of synthetic membranes using biological approaches may yield materials for advanced separations and energy storage.

Capital equipment is provided for such items as advanced nuclear magnetic resonance and magnetic resonance imaging instrumentation and novel atomic force microscopes.

In FY 2007, major activities will include the solar to fuels conversion research with an emphasis on tailoring the absorption and charge separation via the control of photon and electron motion in materials. Such activities will take full advantage of the nanotechnology/biotechnology revolutions to enable exquisite design of materials and the mimicking of natural function. The confluence of the emerging nanoscale hybrid materials and advances in the understanding of nature's design rules of its photosynthetic and catalytic systems opens up opportunities for combining biological and

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

inorganic/organic components in engineered assemblies with unprecedented efficiencies for the conversion of solar photons to fuels and chemicals. Within this activity, there are increases for direct solar conversion to fuels research ($+5,129,000) and for the development of new tools, techniques and mid-scale instrumentation to measure forces, atomic configuration, and physical and chemical properties with ultrahigh sensitivity to further advance nanoscale science ($+1,500,000). Additional funding is provided for research related to the hydrogen economy ($+2,425,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)** | **7,643** | **7,280** | **8,000** |

This activity supports basic research spanning the complete range of activities within the Department in states that have historically received relatively less Federal research funding. The EPSCoR states are Alabama, Alaska, Arkansas, Delaware, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, New Hampshire, Nevada, New Mexico, North Dakota, Oklahoma, Rhode Island, South Carolina, South Dakota, Tennessee, Vermont, West Virginia, Wyoming, the Commonwealth of Puerto Rico, and the U.S. Virgin Islands. The work supported by the EPSCoR program includes research in materials sciences, chemical sciences, biological and environmental sciences, high energy, and nuclear physics, fusion energy sciences, fossil energy sciences, and energy efficiency and renewable energy sciences. In FY 2007, funding is increased for EPSCoR research activities ($+720,000). The following table shows EPSCoR distribution of funds by state.

**EPSCoR Distribution of Funds by State**

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| Alabama | 695 | 685 | 258 |
| Alaska | — | — | — |
| Arkansas | 145 | 135 | 139 |
| Delaware | — | — | — |
| Hawaii | — | — | — |
| Idaho | 476 | 375 | 375 |
| Kansas | 626 | 135 | — |
| Kentucky | 224 | — | — |
| Louisiana | 660 | 462 | 375 |
| Maine | — | — | — |
| Mississippi | 667 | 132 | — |
| Montana | 375 | 455 | 133 |
| Nebraska | 120 | 265 | 269 |
| New Hampshire[a] | — | — | — |
| Nevada | — | 90 | 105 |
| New Mexico | 135 | 135 | — |
| North Dakota | 406 | 273 | — |
| Oklahoma | 485 | 350 | 350 |
| Rhode Island[a] | — | — | — |

[a] Becomes eligible in FY 2006.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Puerto Rico | 375 | 375 | — |
| South Carolina | 716 | 660 | 525 |
| South Dakota | 125 | 125 | — |
| Tennessee | — | 140 | 140 |
| Vermont | 705 | — | — |
| U.S. Virgin Islands | — | — | — |
| West Virgina | 315 | 225 | 135 |
| Wyoming | 270 | 140 | 140 |
| Technical Support | 123 | 60 | 110 |
| Other[a] | — | 2,063 | 4,946 |
| ▪ **Electron-beam Microcharacterization** | **7,614** | **7,945** | **7,945** |

This activity, which was previously budgeted in Structure and Composition of Materials, supports three electron-beam microcharacterization user centers: the Electron Microscopy Center for Materials Research at Argonne National Laboratory, the National Center for Electron Microscopy at Lawrence Berkeley National Laboratory, and the Shared Research Equipment Program at Oak Ridge National Laboratory. These centers contain a variety of highly specialized instruments to provide information on the structure, chemical composition, and properties of materials from the atomic level on up, using direct imaging, diffraction, spectroscopy, and other techniques based primarily on electron scattering.

Atomic arrangements, local bonding, defects, interfaces and boundaries, chemical segregation and gradients, phase separation, and surface phenomena are all aspects of the nanoscale and atomic structure of materials, which ultimately controls the mechanical, thermal, electrical, optical, magnetic, and many other properties and behaviors. Understanding and control of materials at this level is critical to developing materials for and understanding principles of photovoltaic energy conversion, hydrogen production, storage, and utilization, catalysis, corrosion, response of materials in high-temperature, radioactive, or other extreme environments, and many other situations that have direct bearing on energy, environmental, and security issues.

Electron probes are ideal for investigating such structure because of their strong interactions with atomic nuclei and bound electrons, allowing signal collection from small numbers of atoms—or, in certain cases, just one. Furthermore, the use of these charged particles allows electromagnetic control and lensing of electron beams resulting in spatial resolution that can approach single atomic separations or better.

Capital equipment is provided for instruments such as scanning, transmission, and scanning transmission electron microscopes, atom probes and related field ion instruments, related surface characterization apparatus and scanning probe microscopes, and auxiliary tools such as spectrometers, detectors, and advanced sample preparation equipment.

In FY 2007, user operations, scientific research of the staff, and development of new instruments or techniques will continue to be supported at the electron beam microcharacterization user facilities.

[a] Uncommitted funds in FY 2006 and FY 2007 will be competed among all EPSCoR states.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Accelerator and Detector Research** | **4,000** | **2,119** | **3,000** |

This activity supports basic research in accelerator physics and x-ray and neutron detectors. Research seeks to achieve a fundamental understanding beyond the traditional accelerator science and technology to develop new concepts for synchrotron radiation and spallation neutron sources. Research includes studies of the creation and transport of ultra-high brightness electron beams to drive Self Amplified Spontaneous Emission (SASE) Free Electron Lasers (FELs) such as the LCLS. Collective electron effects as micro-bunch instabilities from coherent synchrotron and edge radiation are key areas of interest as they can degrade the beam brightness. In the area of neutron science, there is research to develop improved high intensity, low emittance proton sources in order to achieve high power spallation sources. There is also joint interest in collaboration with NSF on Energy Recovery Linac (ERL) research. There is a coordinated effort between the DOE and NSF to facilitate the development of x-ray detectors. There are ongoing industrial interactions through the SBIR/STTR awards for the development of x-ray detectors.

In the area of neutron science, there is research to develop improved high intensity, low emittance proton sources for accelerator-driven neutron sources. More efficient proton sources can increase the reliability and lifetime due to lower RF power requirements.

To exploit fully the fluxes delivered by synchrotron radiation facilities and the SNS, new detectors capable of acquiring data several orders of magnitude faster than present detectors are required. Improved detectors are especially important in the study of multi-length scale systems such as protein-membrane interactions as well as nucleation and crystallization in nanophase materials. They will also enable real-time kinetic studies and studies of weak scattering samples.

Capital equipment provided for these studies includes lasers for photoionization and laser wake field studies, RF hardware, data acquisition equipment, and optical equipment such as polarizers and beam splitters, interferometers, and specialized cameras.

In FY 2007, activities in novel accelerator and source concepts as well as detector research will continue.

| | | | |
|---|---|---|---|
| ▪ **General Plant Projects** | **3,250** | **—** | **737** |

GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems as part of the BES stewardship responsibilities. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. The total estimated cost of each GPP project will not exceed $5,000,000.

| | | | |
|---|---|---|---|
| ▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor** | **2,000** | **2,000** | **—** |

Capital Equipment funding for new and upgraded instrumentation prior to the installation and commissioning of the cold source has been competed.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Linac Coherent Light Source (LCLS)** | **4,000** | **—** | **—** |

Research and development (R&D) funds were provided to support the physics design of several key LCLS components: the photocathode gun, the linac, the undulator, and the beam optics. These R&D activities were carried out at SLAC and other collaborating institutions in order to reduce the technical risk and provide more confidence in the project's cost and schedule estimates prior to establishing a project performance baseline. No funding is requested in FY 2006 or FY 2007.

| | | | |
|---|---|---|---|
| ▪ **Nanoscale Science Research Centers** | **600** | **993** | **500** |

Funding is provided for Other Project Costs for Nanoscale Science Research Centers.

| | | | |
|---|---|---|---|
| ▪ **The Center for Nanoscale Materials** | **12,000** | **14,000** | — |

Funding was completed in FY 2006 for the Major Item of Equipment with a total estimated cost of $36,000,000 for instrumentation, including clean rooms, for the Center for Nanoscale Materials at Argonne National Laboratory. The instrumentation will be contained in a new building, which was constructed by the State of Illinois at a cost of $36,000,000 and which is dedicated to the Center operations. The building is appended to the Advanced Photon Source. Included within the Center's instrument suite will be an x-ray nanoprobe beamline at the Advanced Photon Source. This beamline will be the highest spatial resolution instrument of its kind in the world, which will permit nondestructive examination of magnetic, electronic, and photonic materials important both for basic science and as foundations for future nanotechnologies.

| | | | |
|---|---|---|---|
| ▪ **Spallation Neutron Source Instrumentation I** | **3,143** | **12,579** | **10,500** |

Funds are provided to continue a Major Item of Equipment with a total estimated cost of $68,500,000 for five instruments for the Spallation Neutron Source that will be installed after the SNS line item project is completed in FY 2006. These instruments will complement the initial suite of five instruments that are being built as part of the SNS construction project, which has capacity for 24 instruments. The instrument concepts for the Major Item of Equipment project were competitively selected using a peer review process. The project will be managed by Oak Ridge National Laboratory with participation by both Argonne and Brookhaven National Laboratories as well as by the State University of New York at Stony Brook. The instruments will be installed at the SNS on a phased schedule between FY 2007 – 2011. A new Major Item of Equipment, described below, will fund approximately four to five additional instruments.

| | | | |
|---|---|---|---|
| ▪ **Research on Instrumentation for the Linac Coherent Light Source (LCLS)** | **1,900** | **1,500** | **—** |

Funding was completed in FY 2006 for research leading to Critical Decision 0 for a Major Item of Equipment for instruments for the Linac Coherent Light Source.

| | | | |
|---|---|---|---|
| ▪ **Transmission Electron Aberration Corrected Microscope (TEAM)** | **5,586** | **6,206** | **5,508** |

Funds are provided for a Major Item of Equipment with a Total Estimated Cost in the range of $11,200,000 to $13,500,000 and a Total Project Cost in the Range of $25,000,000 to $30,000,000. The TEAM project will construct and operate a new aberration-corrected electron microscope and

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

make this capability widely available to the materials and nanoscience communities. The projected improvement in spatial resolution, contrast, sensitivity, and the flexibility of design of electron optical instruments will provide unprecedented opportunities to observe directly the atomic-scale order, electronic structure, and dynamics of individual nanoscale structures. The TEAM instrument will serve as a platform for future aberration-corrected instruments optimized for different purposes such as wide-gap in-situ experimentation, ultimate spectroscopy, ultrafast high-resolution imaging, synthesis, field-free high resolution magnetic imaging, diffraction and spectroscopy, and other extremes of temporal, spectral, spatial or environmental conditions.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)**.................................................................... | **—** | **—** | **10,000** |

Funds are provided for a Major Item of Equipment with a total estimated cost in the range of $50,000,000 to $60,000,000 for four instruments for the Linac Coherent Light source that will be installed after the LCLS line item project is completed in FY 2009. These instruments together with the instrument contained within the LCLS project address all but one of the science thrust areas in the LCLS First Experiments report. The technical concepts for the four instruments have been developed in close consultation with the scientific community through a series of workshops, conferences, and focused review committees. Instrument designs for the Major Item of Equipment project will be competitively selected using a peer review process. The project will be managed by the Stanford Linear Accelerator Complex. The TEC will be narrowed to a cost and schedule performance baseline following completion of Title I design and External Independent Reviews. It is anticipated that these four instruments will be installed at the LCLS on a phased schedule between FY 2009–2012. When completed, the LCLS will provide accommodations for six instrument stations, four of which will be used by the instruments in this Major Item of Equipment.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Spallation Neutron Source Instrumentation II** ....................... | **—** | **—** | **10,000** |

Funds are provided for a Major Item of Equipment with a Total Project Cost in the range of $40,000,000 to $60,000,000 for approximately five instruments for the Spallation Neutron Source that will be installed after the SNS line item project is completed in FY 2006. These instruments will effectively complete the suite of instruments at the SNS. The instrument concepts for the Major Item of Equipment project will be competitively selected using a peer review process. The project will be managed by Oak Ridge National Laboratory. The TEC range will be narrowed to a cost and schedule performance baseline following completion of Title I design and External Independent Reviews. It is anticipated that these instruments will be installed at the SNS on a phased schedule beginning in about FY 2010.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| **Facilities Operations** ......................................................................... | **330,826** | **444,676** | **644,885** |
| ▪ **Operation of National User Facilities**....................................... | **330,826** | **444,676** | **644,885** |

The operations of the scientific user facilities are funded at a level that will permit service to users at optimal capacity, an increase from FY 2006. In addition, funds are provided to partially support operation of the SLAC linac previously fully funded by the High Energy Physics (HEP) program. This marks the second year of a transition of programmatic ownership for SLAC linac operations from HEP to BES as the LCLS project proceeds. FY 2007 funding is requested for National

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|

(dollars in thousands)

Synchrotron Light Source II Other Project Costs for R&D activities to reduce technical risk, including equipment funds for instrumentation required to test prototype components. The Combustion Research Facility is funded in the Chemical Sciences, Geosciences, and Energy Biosciences subprogram at a level that will permit service to users at about the FY 2005 level. The facility operations budget request, presented in a consolidated manner later in this budget, includes operating funds, capital equipment, and accelerator and reactor improvement project (AIP) funding under $5,000,000. AIP funding will support additions and modifications to accelerator and reactor facilities that are supported in the Materials Sciences and Engineering subprogram. General plant project (GPP) funding is also required for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems. The total estimated cost of each GPP project will not exceed $5,000,000. Capital equipment is needed at the facilities for items such as beam monitors, interlock systems, vacuum systems, beamline front end components, monochromators, and power supplies. A summary of the funding for the facilities included in the Materials Sciences and Engineering subprogram is provided below.

## Facilities

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| Advanced Light Source | 44,800 | 42,783 | 49,802 |
| Advanced Photon Source | 100,500 | 95,890 | 108,604 |
| National Synchrotron Light Source | 36,750 | 36,196 | 40,763 |
| National Synchrotron Light Source-II | 1,000 | — | 25,000 |
| Stanford Synchrotron Radiation Laboratory | 32,388 | 25,475 | 35,836 |
| High Flux Isotope Reactor | 46,900 | 43,330 | 51,598 |
| Radiochemical Engineering Development Center | 4,500 | — | — |
| Intense Pulsed Neutron Source | 16,800 | 15,500 | 18,531 |
| Manuel Lujan, Jr. Neutron Scattering Center | 9,588 | 10,000 | 10,582 |
| Spallation Neutron Source | 37,600 | 101,001 | 171,409 |
| Center for Nanophase Materials Sciences | — | 17,800 | 19,190 |
| Center for Integrated Nanotechnologies | — | 11,900 | 19,190 |
| Molecular Foundry | — | 8,100 | 19,190 |
| Center for Nanoscale Materials | — | 3,500 | 19,190 |
| Linac Coherent Light Source (LCLS) | — | 3,500 | 16,000 |
| Linac for LCLS | — | 29,700 | 40,000 |
| Total, Facilities | 330,826 | 444,675 | 644,885 |

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| **SBIR/STTR** | **—** | **18,820** | **24,228** |

In FY 2005, $13,551,000 and $1,626,000 were transferred to the SBIR and STTR programs, respectively. The FY 2006 and FY 2007 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| **Total, Materials Sciences and Engineering** | **621,226** | **737,715** | **1,004,212** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Materials Sciences and Engineering Research** | |
| ▪ **Structure and Composition of Materials** | |
| Increases are provided for developing advanced electron microscopy and scanning probe techniques ($+763,000), research to advance the hydrogen economy ($+100,000), ultrafast science ($+1,000,000), mid-scale instrumentation ($+2,000,000), and solar energy conversion ($+1,439,000) | +5,302 |
| ▪ **Mechanical Behavior and Radiation Effects** | |
| Increase is provided for ongoing research in support of materials related to advanced nuclear reactor fuel cycles | +5,158 |
| ▪ **Physical Behavior of Materials** | |
| Increases are provided for research to advance the hydrogen economy ($+700,000) and solar energy conversion ($+4,379,000). | +5,079 |
| ▪ **Synthesis and Processing Science** | |
| Increase is provided for emergent behavior ($+1,000,000), research to advance the hydrogen economy ($+1,500,000), and solar energy conversion ($+1,439,000) | +3,939 |
| ▪ **Engineering Research** | |
| Termination of selected activities in engineering research including fluid behavior during solidification and heat transfer | -1,444 |
| ▪ **Neutron and X-ray Scattering** | |
| Increases are provided for research and instrumentation for studies of strongly correlated materials, systems at the nanoscale, materials in high fields, and other studies relevant to energy needs ($+9,614,000). Increases are also provided for research to advance the hydrogen economy ($+2,300,000), ultrafast science ($+4,000,000), and mid-scale instrumentation ($+1,000,000) | +16,914 |
| ▪ **Experimental Condensed Matter Physics** | |
| Increases are provided for research to advance the hydrogen economy ($+3,350,000), mid-scale instrumentation ($+2,500,000), and solar energy conversion ($+4,939,000) | +10,789 |
| ▪ **Condensed Matter Theory** | |
| Increases are provided for research to advance the hydrogen economy ($+1,100,000), emergent behavior ($+1,500,000), and solar energy conversion ($+1,920,000) | +4,520 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Materials Chemistry** | |
| Increases are provided for research to advance the hydrogen economy ($+2,425,000), mid-scale instrumentation ($+1,500,000), and solar energy conversion ($+5,129,000) | +9,054 |
| ▪ **Experimental Program to Stimulate Competitive Research (EPSCoR)** | |
| Increases is provided for additional EPSCoR research activities | +720 |
| ▪ **Accelerator and Detector Research** | |
| Increase is provided for additional research in new accelerator and detector concepts, including accelerator concepts for light sources not necessarily based on storage-ring technologies | +881 |
| ▪ **General Plant Projects** | |
| Increase is provided for general plant projects as part of the BES stewardship responsibilities | +737 |
| ▪ **Neutron Scattering Instrumentation at the High Flux Isotope Reactor** | |
| Funding for new and upgraded instrumentation prior to installation and commissioning of the cold source is complete.. | -2,000 |
| ▪ **Nanoscale Science Research Centers** | |
| Scheduled decrease for Other Project Costs for the Nanoscale Science Research Centers. Funding is provided for Other Project Costs for the BNL Center for Functional Nanomaterials. No Other Project Costs are required for the remaining Nanoscale Science Research Centers | -493 |
| ▪ **The Center for Nanoscale Materials** | |
| Scheduled decrease for the Major Item of Equipment for the ANL Center for Nanoscale Materials due to its completion | -14,000 |
| ▪ **Spallation Neutron Source Instrumentation I** | |
| Scheduled decrease for Instrumentation for the Spallation Neutron Source. | -2,079 |
| ▪ **Research on Instrumentation for the Linac Coherent Light Source (LCLS)** | |
| Scheduled decrease for R&D on instrumentation for the LCLS | -1,500 |
| ▪ **Transmission Electron Aberration Corrected Microscope (TEAM)** | |
| Scheduled decrease for the Major Item of Equipment for the Transmission Electron Aberration Corrected Microscope | -698 |
| ▪ **Linac Coherent Light Source Ultrafast Science Instruments (LUSI)** | |
| Initiate Major Item of Equipment for approximately four instruments at the Linac Coherent Light Source. | +10,000 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Spallation Neutron Source Instrumentation II** | |
| Initiate a new Major Item of Equipment for approximately four to five additional instruments for the Spallation Neutron Source | +10,000 |
| **Total, Materials Sciences and Engineering Research** | **+60,879** |
| **Facilities Operations** | |
| ▪ **Operation of National User Facilities** | |
| Increase for the Advanced Light Source to support accelerator operations and for increased support for users | +7,019 |
| Increase for Advanced Photon Source to support accelerator operations and for increased support for users | +12,714 |
| Increase for National Synchrotron Light Source to support accelerator operations and for increased support for users | +4,567 |
| Increase for National Synchrotron Light Source-II – Other Project Costs per FY 2007 project data sheet | +25,000 |
| Increase for the Stanford Synchrotron Radiation Laboratory to support accelerator operations and for increased support for users | +10,361 |
| Increase for High Flux Isotope Reactor to support reactor operations | +8,268 |
| Increase for Intense Pulsed Neutron Source to support accelerator operations and for increased support of users. | +3,031 |
| Increase for the Manuel Lujan, Jr., Neutron Scattering Center to support target operations and for increased support for users | +582 |
| Increase for Spallation Neutron Source to support operations in the first full year of operation. | +70,408 |
| Increase for the Center for Nanophase Materials Sciences for continued operations. | +1,390 |
| Increase for Center for Integrated Nanotechnologies for continued operations | +7,290 |
| Increase for Molecular Foundry for continued operations. | +11,090 |
| Increase for Center for Nanoscale Materials for continued operations. | +15,690 |
| Increase for Linac Coherent Light Source Other Project Costs per FY 2007 project datasheet. | +12,500 |
| Increase for Stanford Linear Accelerator Center in support of the linac operations | +10,300 |
| **Total, Facilities Operations** | **+200,210** |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **SBIR/STTR** | |
| Increase in SBIR/STTR funding because of an increase in total operating expense.......... | +5,408 |
| **Total Funding Change, Materials Sciences and Engineering** ....................................... | **+266,497** |

# Chemical Sciences, Geosciences, and Energy Biosciences

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Chemical Sciences, Geosciences, and Energy Biosciences | | | |
| Chemical Sciences, Geosciences, and Energy Biosciences Research | 225,928 | 208,831 | 255,113 |
| Facilities Operations | 6,437 | 6,251 | 6,805 |
| SBIR/STTR | — | 5,468 | 6,581 |
| Total, Chemical Sciences, Geosciences, and Energy Biosciences | 232,365 | 220,550 | 268,499 |

### Description

This subprogram provides support for basic research in atomic, molecular and optical science; chemical physics; photochemistry; radiation chemistry; physical chemistry; inorganic chemistry; organic chemistry; analytical chemistry; separation science; heavy element chemistry; geochemistry; geophysics; and physical biosciences.

Included within the $255,113,000 research component of this subprogram is support for General Plant Projects and General Purpose Equipment totaling $17,466,000.

### Benefits

Ultimately, research in chemical sciences leads to the development of such advances as efficient combustion systems with reduced emissions of pollutants; new solar photoconversion processes; improved catalysts for clean and efficient production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. Research in geosciences contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance. Research in biosciences provides the foundation for new biological, biomimetic, and bioinspired paths to solar energy conversion, fuels and chemical feedstock production, chemical catalysis, and materials synthesis.

### Supporting Information

This research seeks to understand chemical reactivity through studies of the interactions of atoms, molecules, and ions with photons and electrons; the making and breaking of chemical bonds in the gas phase, in solutions, at interfaces, and on surfaces; and energy transfer processes within and between molecules. In geosciences, support is provided for mineral-fluid interactions; rock, fluid, and fracture physical properties; and new methods and techniques for geosciences imaging from the atomic scale to the kilometer scale. In the area of biosciences, support is provided for molecular-level studies on solar energy capture through natural photosynthesis; the mechanisms and regulation of carbon fixation and carbon energy storage; the synthesis, degradation, and molecular interconversions of complex hydrocarbons and carbohydrates; and the study of novel biosystems and their potential for materials synthesis, chemical catalysis, and materials synthesized at the nanoscale.

This subprogram provides support for chemistry comparable to that of the National Science Foundation. It is the Nation's sole support for heavy-element chemistry, and it is the Nation's primary support for homogeneous and heterogeneous catalysis, photochemistry, radiation chemistry, separations and analysis, and gas-phase chemical dynamics.

**Selected FY 2005 Research Accomplishments**

- Timing the World's Shortest X-Ray Pulses. Light sources based on particle accelerators, such as the Linac Coherent Light Source (LCLS), will revolutionize x-ray science due to their unprecedented brightness and extremely short pulse duration. To take full advantage of x-ray pulses that last only a few femtoseconds ($10^{-15}$ seconds), they must be timed relative to equally short pulses from an optical laser. Such measurements are vital to a wide range of LCLS experiments in which a sample is excited by an optical pulse and probed by an x-ray pulse. At the Stanford Linear Accelerator Center, ultrashort x-ray pulses were generated when 80-femtosecond electron pulses from an accelerator were sent through an undulator magnet; the x-ray and electron pulses were perfectly coincident in time. A crystal placed near the path of the electron beam experienced intense electric fields that altered the optical properties of the crystal, the electro-optic (EO) effect. An optical laser beam passing through the crystal sensed the EO effect, turning the time delay between the optical pulse and the electron/x-ray pulse into a spatial displacement on a detector. The current timing resolution of 60 femtoseconds could be improved to 5 femtoseconds, matching the projected performance of accelerator-based light sources into the foreseeable future.
- Molecular Fragmentation Observed in Unprecedented Detail. Researchers working at the Advanced Light Source have advanced our ability to observe the total destruction of a molecule to new levels of sophistication, challenging theoretical understanding and paving the way for research to be performed at next-generation light sources. When a hydrogen molecule is exposed to x-ray photons of the appropriate energy, the two electrons it possesses can be ejected at once, leaving behind two positively charged nuclei that rapidly explode. Thus, absorption of one x-ray photon causes the complete destruction of the molecule. Using modern techniques of three-dimensional imaging and ultrafast timing, the motions of all four particles from a single event can be related to one another. The results are surprising and challenge our current theoretical understanding of how x-rays interact with matter.
- Complete Ionization of Clusters in Intense VUV Laser Fields. BES-supported researchers have developed a theory that explains recently-observed ionization behavior of xenon clusters that were exposed to intense, coherent vacuum ultraviolet (VUV) pulses from a free-electron laser (FEL). Surprisingly, at intensities that produce only single ionization of an isolated xenon atom, the clusters irradiated by the FEL showed massive ionization in which every atom in the cluster was highly ionized, producing ions with charge states up to +8. This implies that each xenon atom in the cluster absorbed about 30 VUV photons. The key difference between clusters and isolated atoms is that energetic electron-ion collisions occur within the clusters and modify the single-photon absorption cross section, thus allowing a large number of photons to be absorbed. This process is called "inverse bremsstrahlung" and, when incorporated into a simple linear absorption model, clearly reproduces the experimental observations. Theories such as this will be needed to understand the behavior of matter when it is exposed to intense, coherent X-ray pulses from next-generation light sources such as the LCLS.
- The Roaming Atom: Straying from the Lowest-energy Reaction Pathway. A fundamental tenet of modern chemical reaction theory is the concept of the transition state, a transient molecular entity

that lies on the most direct pathway from reactants to products and whose properties govern the rate of reaction. Recently, it was shown that in a simple chemical reaction, the decomposition of formaldehyde, a substantial fraction of the dissociating molecules avoid the region of the transition state entirely. These studies combine ion imaging experiments with theoretical trajectory calculations to reveal that the dissociation takes place via a mechanism in which one hydrogen atom begins to roam away from the molecule and nearly dissociates, then returns to react with the remaining hydrogen atom. Along with other recent findings on reactions such as $O + CH_3$, these results challenge conventional notions of chemical reactions and raise the question of how common such processes might be. A key question is whether such a mechanism applies only to reactions forming hydrogen, during which a light hydrogen atom may rapidly explore regions far from the conventional transition state.

- New Combustion Intermediates Discovered. A complete mechanism for the combustion of simple hydrocarbon fuels includes dozens of distinct molecular species and hundreds of chemical reactions. The identification of which molecules to include in a combustion chemistry mechanism still requires experimental detection, particularly for reactive intermediates. A class of unstable molecules known as enols, which have OH groups adjacent to carbon-carbon double bonds, are not currently included in standard combustion models. In work performed at the Advanced Light Source, significant quantities of 2, 3, and 4-carbon enols were observed using photoionization mass spectrometry of flames burning representative compounds from modern fuels. Concentration profiles of the enols taken in the model flames demonstrate that their presence cannot be accounted for by isomerization reactions that convert more stable molecules into enols. This leads to the conclusion that an entire class of important reaction intermediates is absent from current combustion models, and the models will need substantial revision.
- Unified Molecular Picture of the Surfaces of Aqueous Solutions. A long-term controversy exists regarding the detailed, molecular nature of the surface of an aqueous solution containing molecular ions (or electrolytes). Joint theoretical and experimental studies have led to a new, unified view of the structure of the interface between air and aqueous electrolytes. Molecular dynamics simulations have shown that in basic salt solutions positively charged ions (cations) are repelled from the interface, while negatively charged ions (anions) exhibit a propensity to migrate toward the surface that correlates with the anion's polarizability and physical size. In acidic solution, however, there is a high propensity for cations to be located at the air/solution interface. In this case, both cations and anions are concentrated at the surface and reduce the surface tension of water. These conclusions have been verified by surface-selective nonlinear vibrational spectroscopy experiments. Understanding the behavior of ions at aqueous surfaces is important to the heterogeneous chemistry of seawater aerosols and to the tropospheric ozone destruction in the Arctic and Antarctic due to reactions on ice pack covered with sea spray.
- Self-Assembled Artificial Photosynthesis. In natural photosynthesis, self-assembly of light-absorbing molecules, or chromophores, at specific distances and orientations is especially important in two parts of the overall photosynthetic system: the antenna component, where light is collected; and the reaction center, where charge is separated. Recently, a green organic chromophore was discovered that exhibits photophysical and photoredox properties similar to those of natural chlorophyll a. When conjoined with four similar chromophores, the molecules self-assemble in solution to form an antenna-reaction center complex. Self-organization of the large structure is believed due to the propensity of these similar chromophores to align in a cofacial stacking arrangement. The self-

assembled organic has attributes that closely mimic the primary events in photosynthesis: efficient light energy capture over a wide spectral range, energy funneling toward a core electron-transferring unit, and excited-state symmetry breaking of a molecular pair resulting in charge separation. The structure of the new array was determined at the Advanced Photon Source.

- Two-Dimensional Spectroscopy Reveals Energy Transport Pathways In Photosynthesis. Photosynthetic antennas capture solar photons and transport the absorbed energy to the photosynthetic reaction center where charge separation occurs. Energy transfer by the antenna is nearly 100 percent efficient, although the mechanism for the process has been elusive. A novel spectroscopic technique known as a two-dimensional photon echo, commonly used in the infrared, has been extended to the visible spectral region and has revealed important details about energy transfer in photosynthetic light harvesting. In antenna pigments from green sulfur bacteria, distinct energy transport pathways have been identified that depend on the spatial properties of the pigment-protein complex. Contrary to the accepted model of a sequential cascade in energy from high- to low-lying excited states, these results reveal excited states that are distributed over two or more chlorophyll molecules and a pathway in which energy levels are skipped on the way to the lowest level. The new two-dimensional electronic spectroscopic method, which measures electronic couplings and maps the flow of excitation energy, opens the door to investigation of other photoactive systems and can be applied to improving the efficiency of molecular solar cells.
- How Water Networks Accommodate an Excess Electron. In bulk water an excess electron can become trapped within a cavity formed by a network of hydrogen-bonded water molecules. This "solvated electron" is a critical chemical intermediate in the radiolysis of aqueous solutions. One approach to understanding the solvated electron is to study the structure and dynamics of clusters of water containing an excess electron in the gas phase. This approach has not yet been successful because these anionic water clusters are hard to make and because an accurate theoretical description for them is lacking. Recent work has shown that anionic clusters containing four to six water molecules can be created within gas-phase matrices of inert argon clusters, where their infrared spectra can be obtained. Analysis of these spectra using density functional theory shows that the diffuse electron interacts most strongly with a single water molecule that is hydrogen bonded to two other waters in a rearranged network. The spectra also exhibit evidence for the rapid exchange of energy between the vibrations of the hydrogen atoms on the unique molecule and the excess electron. This new technique can now be extended to larger water clusters that better mimic the solvated electron in bulk water.
- Gold, a Magnificent Nanoscale Catalyst. When gold atoms are assembled as tiny clusters smaller than 8 nanometers and attached to the surface of titanium oxide, they acquire the remarkable ability to dissociate oxygen at room temperature and insert that oxygen into very specific locations in molecules. The origin of such unusual reactivity—discovered some 10 years ago—has until recently evaded a widely accepted explanation. Numerous parameters in the material are important and usually cross-correlated: gold particle dimension and shape, metal oxidation state, oxide support reducibility, and interaction of the gold with the support. Separating those parameters in these materials, which are macroscopically amorphous, would demand special analytical techniques that are able to focus on the detailed properties of individual chemical bonds in the solid. Therefore, researchers pursued a different route using existing and well-known surface science techniques: they accurately synthesized and stacked one-atom-thick layers of gold extended in two dimensions, and supported them on top of perfect oxide crystals of known structure. They demonstrated that the

nanoscale properties of gold metal are achievable by controlling the layer thickness to between 2 and 3 atoms. Such knowledge can now be extended to the manipulation of selective oxidation chemistry or the discovery and assembly of new catalysts.

- Theory Guides Scientists on How to Extract Hydrogen from Natural Sources and Store it Efficiently. Two of the keys to a hydrogen economy are having an abundant supply of hydrogen and having materials that can store such hydrogen in a readily accessible form. Both of those challenges can be addressed by designing materials—chemical catalysts—that bind atomic hydrogen with medium strength and release molecular or gaseous hydrogen with very little heating. A random or systematic search for such catalysts, even with high-throughput techniques, would be very expensive and take many years. Scientists resorted to so-called density-functional theory, which is an electronic structure theory of matter, and other theories that describe chemical reactivity to design the ideal bimetallic catalysts, combinations of two metals, in special atomic arrangements that would result in solids with the desired properties. They arrived at a new theoretical construct called near-surface alloys of metals, such as a crystal of platinum containing a single layer of nickel atoms in its second row, that possesses the unique catalytic behavior sought. Having by now mapped entire families of such new theoretical materials—a feat unachievable by direct experimental means—these scientists have embarked on the challenge of fabricating these new structures and have already demonstrated their concept with a few successful examples.
- Devising the Next-Generation Wonder Molecules—Fine Chemistry inside Nano Cages. In the future drugs, fibers, fuel additives, molecular electronics devices, solar energy conversion dyes, and flavors may be synthesized in a similar manner using sets of discrete cavities to contain and isolate single molecules or just reacting pairs of molecules and catalysts. The “single-molecule catalysis” concept would allow maximum control of the environment surrounding a molecule, the spatial arrangement adopted by its atoms, the type of bonds made available for reaction, and even how the energy is coupled to and transferred to the molecule. Such level of control would result in the ability to break bonds or insert or remove atoms or change the spatial arrangement of atoms in very specific ways and not others. The resulting products would possess properties—chemical, biological, optical, electronic, or mechanical—superior to those achievable through less controllable chemistry. Researchers are beginning to show that this goal may be achievable. So-called supramolecular or larger-than-molecules cages made with organometallic compounds were used to host other organometallic complexes that have catalytic properties, such as the ability to specifically break carbon-hydrogen bonds. They have shown that certain carbon-hydrogen bonds are selectively broken and that only certain members of a chemical family undergo reaction, and not others. They have even shown that the constrained environment also leads to enhanced rate of production of the most desired product, which is in itself a revolutionary discovery.
- Controlling the Crash-landing of Biomolecules on Surfaces. Researchers have, for the first time, demonstrated that peptide ions retain at least one proton after soft landing on chemically modified, “fluffy” surfaces. Controlled deposition on surfaces holds great potential for applications such as selective chemical separations and analysis. Soft landing refers to the intact capture of large size-selected, charged molecules on surfaces of liquids or solids. Previous research suggests that soft landing provides a means for highly specific deposition of molecules of any size and complexity on surfaces using only a tiny fraction of material normally used in standard synthetic approaches. In the present studies, peptide ions are attractive as model systems that can provide important insights on the behavior of soft-landed macromolecules. The researchers used a specially designed mass

spectrometer configured for studying interactions of large ions with surfaces. The special characteristics of the instrument enabled quantitative investigation of the effect of the speed and mass of ions on the soft landing process. For example, it was determined that even collisions with high energies can result in deposition of intact ions on surfaces.

- Removal of Radium Ions from Water using Special "Grabber" Molecules. Researchers demonstrated a process that is highly selective for binding radium cations. It is a significant challenge to remove radioactive radium cations from wastewater since the large excess of other non-radioactive ions in solution can interfere with the selective extraction of radium. In the new work, a specially designed molecule was used to selectively bind radium. This supramolecular assembly made from isoguanosine is just the right size to extract radium in the presence of other cations such as magnesium and sodium.
- How Molecules Move through Small Holes. Measurements of transport through 15-nanometer pores have been compared to theoretical results to yield new understanding of differential transport at small scales. This knowledge is important for an understanding of separation processes at the molecular level, and could lead to a new generation of analytical devices based on microfluidic platforms. By adjusting physical parameters such as the channel diameter, and applying the appropriate external electrical potential, arrays of nanochannels—formed by nanocapillary array membranes—can be made to behave like digital fluidic switches, and the movement of molecules from one side of the array to the other side can be controlled. Combining model calculations with experimental characterization provides important insights into the mechanism of molecular transport and, additionally, provides quantitative measures of the surface characteristics of the interior of the pores.
- Using Thorium and Uranium to Activate the Carbon-Hydrogen and Carbon-Nitrogen Bonds in Molecules. The extent of electron-sharing in bonds with metals is an important property in catalysis. The correlation of bond covalency with reactivity can be elucidated by determining the reactivity of actinide (thorium, uranium, and other elements in the same row of the periodic table) ions with multiply bonded functional groups. Pyridine N-oxide ($C_5H_5N$-O), which has a relatively stable benzene-like ring, can transfer oxygen atoms to certain transition metals. Chemists have discovered that some uranium and thorium compounds can make C-H bonds in pyridine N-oxide more reactive by forming metal-carbon bonds. The structures of the products produced in these new reactions have been confirmed by x-ray crystallography. These reactions provide examples of C-H and C=N bond activation that is mediated by actinide metals. These studies may offer insights into catalytic removal of nitrogen-containing compounds from petroleum feedstocks, which is necessary to reduce nitrogen oxide emission in fuels.
- Elusive Carbon Dioxide Binding Mode Discovered in New Uranium Complex. Carbon dioxide ($CO_2$) is a stable molecule with two strong carbon-oxygen bonds. Inorganic chemists seek to mimic the catalytic chemical processes by which carbon dioxide is modified by plants to form sugars. This process can remove $CO_2$ from the atmosphere and minimize atmospheric release of $CO_2$ in industrial processes such as refinement of hydrocarbons. A new exquisitely-designed uranium complex has been found to react with $CO_2$ such that one electron is transferred from the $U^{3+}$ center to $CO_2$, producing a species with an unusual linear $CO_2$ that binds to uranium and has one weaker oxygen-carbon bond. Uranium is an essential component of this species because the $U^{3+}$ ion is large, electron-rich, and has the right structure to participate in bonding. This species is unique in that the $CO_2$ remains linear, with one C-O bond longer and weaker than the other. The molecular structure,

bond lengths and oxidation state were established experimentally. The linear M-O-C-O coordination had previously been seen only in an iron enzyme. The new uranium-$CO_2$ complex represents a chemical image of a catalytic process and may make it possible to design new catalysts to reduce the concentration of $CO_2$ in the atmosphere.

- Plutonium is Caged and Illuminated by Synchrotron Light. A new complexant, which was synthesized to extract plutonium and other actinide elements selectively, has shown promise to remove plutonium from mammals. Microscopic crystals (about the thickness of a human hair) of a plutonium complex have been produced to provide a structural model in order to design new actinide-selective binders. Using the Advanced Light Source, researchers determined the detailed structure of these crystals and showed that individual plutonium ions are trapped in cavities produced by eight oxygen atoms from the binder molecules. This structural determination will serve as a model of such complexes on which to base the design of novel molecules that are cages for toxic metals.
- Sheer Energy: Thinner, Cheaper Fuel Cell Catalysts. Fuel cells are a major source of clean energy in the hydrogen economy. Their economic development critically depends on cheaper electrocatalysts for oxygen reduction. The slow nature of this reaction causes a major limit in fuel cell efficiency. High precious metal content is another drawback of existing technology. Researchers coated five cheaper metals with a layer of platinum one atom thick and tested them. For most of the platinum "monolayers," the reaction occurred more slowly than it does on the thicker platinum layer currently used in fuel cells. But adding a monolayer of platinum to the cheaper metal palladium sped up the reaction. Theoretical computations predicted how the platinum monolayers are affected by atoms from the underlying layer of metal. The theory agreed well with the experiments and showed that a platinum monolayer on palladium balances two competing needs: it is reactive enough to break the bonds between oxygen atoms yet does not cling to the oxygen atoms so tightly that it prevents them from reacting with hydrogen. This method can dramatically decrease the expensive metal loading in fuel cells and improve cost and performance.
- Advances in Computational Chemistry Research. Basic research in computational chemistry has resulted in a superior method for the prediction of chemical behavior from computational quantum mechanics and statistical mechanics. The method is based on treating the solvent in which a molecule is placed as a continuum, and determining the cavity-formation energy from statistical mechanics, and the electric contributions from quantum mechanics. This work has now been published and a leading chemical process simulation company has incorporated this method into the most recent release of their industry dominating process simulator. This work will impact modern industrial plant and process design and lead to higher energy efficiencies through effective modeling of manufacturing processes.
- Is $CO_2$ Gone When You Put It In The Ground? There are only two options for dealing with increasing $CO_2$ concentrations in the atmosphere—get rid of new $CO_2$ actively or discontinue producing it and wait for natural processes to remove the excess over a very long time. Both approaches will likely be needed in the future. Researchers have been developing capabilities for realistic modeling of $CO_2$ injection into deep geological formations and for understanding dynamic processes associated with the injection in order to provide a scientific basis for evaluating the injections feasibility. Computational models were developed for coupling fluid properties, chemical and thermodynamic data, and rock-fluid interaction measurements. Reservoir dynamics were investigated on different levels of complexity and scale for natural and engineered systems. These

types of calculations also form the basis for understanding possible leaks which may be major regulatory and insurance concerns for large scale geological $CO_2$ sequestration. The improved computational codes from this project were also used as the basis for design calculations for $CO_2$ injection at the Frio Test Site as part of the Office of Fossil Energy funded Climate Change Technology Program.

- Improving Our Vision of the Subsurface. Large scale subsurface seismic measurements, although adequate for simple oil and gas exploration or waste site characterization, are inadequate for high hydrocarbon recovery rates or more effective environmental remediation or monitoring. Research is providing a better understanding of geophysical measurements of compressional and shear wave velocities, elastic moduli, and seismic anisotropy as they vary as functions of porosity, permeability, fluid contents, and stresses. A fiber-optic "optical" strainmeter has been developed that provides spatially averaged properties over a centimeter or "core" length scale intermediate between point measurements and a meter-scale bulk-measurements. The increased accuracy and sensitivity in measuring elastic deformation during applied sinusoidal stress will enable better discrimination between strain (elastic wave transmission efficiency) and phase lags (attenuation indicative of fluid content and type). In addition, the highly precise optical strain gage measurements will allow higher resolution testing of the significance of different types of heterogeneity at the core scale, in order to enable prediction of these properties at larger scales. The fiber optic sensor has been demonstrated to have a significantly higher sensitivity than other strain gages.

- The Auxin Receptor: A Holy Grail in Plant Science. The plant growth hormone called auxin is a small molecule, indole acetic acid (IAA)—too small to have the expected breadth of "informational" content to achieve its myriad effects of controlling the growth of leaves, stems, roots, flowers, fruits, and growth changes in response to light and gravity. Recent research demonstrated that IAA interacts directly with a much larger molecule, a protein, which was earlier shown to affect plant growth by stimulating the expression (activation) of certain growth-related genes. Now the solution to the mystery of auxin action is becoming clear. It turns out to be similar to an electric switch, but a bit more complex. We are beginning to unravel the molecular details of auxin's biological activity.

## Detailed Program Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Chemical Sciences, Geosciences, and Energy Biosciences Research** | **225,928** | **208,831** | **255,113** |
| ▪ **Atomic, Molecular, and Optical (AMO) Science** | **16,627** | **15,397** | **19,248** |

This activity supports theory and experiments to understand the properties of and interactions among atoms, molecules, ions, electrons, and photons. Included among the research activities are studies to determine the quantum mechanical description of such properties and interactions; interactions of intense electromagnetic fields with atoms and molecules; development and application of novel x-ray light sources; the development of new ultrafast optical probes; and ultracold collisions and quantum condensates.

The knowledge and techniques developed in this activity have wide applicability. Results of this research provide new ways to use photons, electrons, and ions to probe matter in the gas and

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

condensed phases. This has enhanced our ability to understand materials of all kinds and enables the full exploitation of the BES synchrotron light sources, electron beam micro-characterization centers, and neutron scattering facilities. Furthermore, by studying energy transfer within isolated molecules, AMO science provides the very foundation for understanding chemical reactivity, i.e., the process of energy transfer between molecules and ultimately the making and breaking of chemical bonds. The AMO Science activity is the sole supporter of synchrotron-based AMO science studies in the U.S., which includes ultrashort x-ray pulse generation and utilization at the ALS and APS. This program is also the principal U.S. supporter of research in the properties and interactions of highly charged atomic ions, which are of direct consequence to fusion plasmas.

Capital equipment is provided for items including lasers and optical equipment, unique ion sources or traps, position sensitive and solid-state detectors, and control and data processing electronics.

In FY 2007, major activities will include the interactions of atoms and molecules with intense laser pulses; the development of new ultrafast optical probes and theories for the interpretation of ultrafast measurements; the use of optical fields to control quantum mechanical processes; atomic and molecular interactions at ultracold temperatures; and the creation and utilization of quantum condensates that provide strong linkages between atomic and condensed matter physics at the nanoscale. Within this funding, there are increases for coherent control of quantum systems ($+851,000), ultrafast science ($+2,000,000), chemical imaging ($+500,000), and mid-scale instrumentation ($+500,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Chemical Physics Research** ........................................................ | **32,946** | **31,866** | **37,813** |

This activity supports experimental and theoretical investigations of gas phase chemistry and chemistry in the condensed phase and at interfaces. Gas phase chemistry emphasizes the dynamics and rates of chemical reactions characteristic of combustion with the aim of developing theories and computational tools for use in combustion models and experimental tools for validating these models. The study of chemistry in the condensed phase and at well characterized surfaces and the reactions of metal and metal oxide clusters lead to the development of theories on the molecular origins of surface mediated catalysis.

This activity also has oversight for the Combustion Research Facility (which is budgeted below in Facilities Operations), a multi-investigator facility for the study of combustion science and technology. In-house BES-supported efforts combine theory, modeling, and experiment including diagnostic development, kinetics, and dynamics. Several innovative non-intrusive diagnostics have been developed to characterize gas-phase processes, including high-resolution optical spectroscopy, time-resolved Fourier transform infrared spectroscopy, picosecond laser-induced fluorescence, and ion-imaging. Other activities at the Combustion Research Facility involve BES interactions with Fossil Energy, Energy Efficiency and Renewable Energy, and industry.

This activity contributes significantly to DOE missions, since nearly 85% of the Nation’s energy supply has its origins in combustion and this situation is likely to persist for the foreseeable future. The complexity of combustion—the interaction of fluid dynamics with hundreds of chemical reactions involving dozens of unstable chemical intermediates—has provided an impressive challenge to predictive modeling of combustion processes. Predicted and measured reaction rates will be used in models for the design of new combustion devices with maximum energy efficiency and minimum undesired environmental consequences.

The research in chemical dynamics at surfaces is aimed at developing predictive theories for surface mediated chemistry such as is encountered in industrial catalysis or environmental processes. Surface mediated catalysis reduces the energy demands of industrial chemical processes by bypassing energy barriers to chemical reaction. Surface mediated catalysis is used to remove pollutants from combustion emissions.

The SciDAC computational chemistry program addresses two fundamental research efforts: (1) chemically reacting flows and (2) the chemistry of unstable species and large molecules. Each of these research efforts is carried out by a team of related scientists working with the appropriate Integrated Software Infrastructure Centers supported under SciDAC by the SC Advanced Scientific Computing Research program.

Capital equipment is provided for such items as picosecond and femtosecond lasers, high-speed detectors, spectrometers, and computational resources.

In FY 2007, there will be an increased emphasis on chemical physics in the condensed phase, including the fundamental understanding of weak, non-covalent interactions and their relationship to chemical and physical properties of macroscopic systems, and on electron driven chemical reactions at interfaces relevant to solar energy conversion. Within this funding, there are increases for condensed phase and interfacial molecular science ($+1,000,000), ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), and solar energy conversion ($+1,697,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Photochemistry and Radiation Research**................................ | **30,446** | **25,489** | **32,007** |

This activity supports fundamental molecular level research on the capture and conversion of energy in the condensed phase. Fundamental research in solar photochemical energy conversion supports organic and inorganic photochemistry, and photocatalysis photoinduced electron and energy transfer in the condensed phase, photoelectrochemistry, biophysical aspects of photosynthesis, and biomimetic assemblies for artificial photosynthesis. Fundamental research in radiation chemistry supports chemical effects produced by the absorption of energy from ionizing radiation. The radiation chemistry research encompasses heavy ion radiolysis, models for track structure and radiation damage, characterization of reactive intermediates, radiation yields, and radiation-induced chemistry at interfaces. Accelerator-based electron pulse radiolysis methods are employed in studies of highly reactive transient intermediates, and kinetics and mechanisms of chemical reactions in the liquid phase and at liquid/solid interfaces. This activity supports the Notre Dame Radiation Laboratory, a BES collaborative research center, emphasizing research in radiation chemistry.

Solar photochemical energy conversion is a long-range option for meeting future energy needs. An alternative to semiconductor photovoltaic cells, the attraction of solar photochemical and photoelectrochemical conversion is that fuels, chemicals and electricity may be produced with minimal environmental pollution and with closed renewable energy cycles. Artificial photosynthesis can be coupled to chemical reactions for generation of fuels such as hydrogen, methane, or complex hydrocarbons found in gasoline. The fundamental concepts devised for highly efficient excited-state

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

charge separation in molecule-based biomimetic assemblies should also be applicable in the future development of molecular optoelectronic devices. A strong interface with the Office of Energy Efficiency and Renewable Energy (EE) solar conversion programs exists at National Renewable Energy Laboratory (NREL), involving shared research, analytical and fabrication facilities, and involving a jointly shared project on dye-sensitized solar cells.

Radiation chemistry research supports fundamental chemical effects produced by the absorption of energy from ionizing radiation. This research is important for solving problems in environmental waste management and remediation, nuclear energy production, and medical diagnosis and radiation therapy.

This activity is the dominant supporter (85%) of solar photochemistry in the U.S., and the sole supporter of radiation chemistry.

Capital equipment is provided for such items as pico- and femtosecond lasers, fast Fourier transform-infrared and Raman spectrometers, and upgrades for electron paramagnetic resonance spectroscopy.

In FY 2007, funding will include research to expand our knowledge of the semiconductor/liquid interface, colloidal semiconductors, and dye-sensitized solar cells; inorganic/organic donor-acceptor molecular assemblies and photocatalytic cycles; photosynthetic antennae and the reaction center; the use of nanoscale materials in the photocatalytic generation of hydrogen from water and other fuels from fossil feedstocks; and radiolytic processes at interfaces, radiolytic intermediates in supercritical fluids, and characterization of excited states by dual pulse radiolysis/photolysis experiments. Within this funding, there are increases for ultrafast science ($+1,000,000), solar energy conversion ($+3,909,000), and research related to the hydrogen economy ($+1,609,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Molecular Mechanisms of Natural Solar Energy Conversion** | **13,640** | **12,411** | **18,188** |

This activity supports fundamental research at the interface between the biological and physical sciences to characterize the molecular and chemical mechanisms involved in the conversion of solar energy to stored chemical energy. Research supported includes the characterization of the chemical processes occurring during photosynthesis, the kinetic and catalytic mechanisms of enzymes involved in the synthesis chemical fuels, and the biochemical mechanisms involved in the fixation of carbon dioxide. The approaches used include biophysical, biochemical, and molecular structure/function analyses. The goal is to enable the future biotechnological exploitation of both natural and synthetic systems and to provide insights and strategies into the design of non-biological and hybrid processes. This activity encourages fundamental research that employs novel approaches that integrate biological sciences with physical sciences in order to understand the molecular details of energy conversion by natural systems.

Capital equipment is provided for such items as high-speed lasers, high-speed detectors, spectrometers, and computational resources.

In FY 2007, funding will support research that focuses on understanding the constituents and molecular-level interactions within natural photosynthetic systems and the detailed molecular processes associated with the absorption of solar energy and the creation of stored chemical energy.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

Exploiting and mimicking components of natural solar energy conversion will enable future strategies for the bio-inspired design of new energy capture systems. Within this funding, there are increases for biophysical characterization of biomolecular complexes ($+500,000), chemical imaging ($+750,000), emergent behavior ($+500,000) solar energy conversion ($+3,909,000), and research related to the hydrogen economy ($+118,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Metabolic Regulation of Energy Production** ........................ | **19,427** | **17,554** | **17,601** |

This activity supports fundamental research in the molecular processes that constitute and regulate metabolic pathways that are involved in cellular chemical conversions of importance to energy. Understanding the molecular mechanisms of chemical transformations and the control of chemical transformation pathways in living systems, such as plants, provides the basis for modifying biological processes and designing bioinspired, synthetic systems for applications in energy technologies. The research goal is to develop a predictive and experimental context for the manipulation of metabolism to accumulate a desired product and to design and synthesize robust bioinspired and biomimetic systems, including hybrid systems that achieve desired chemical transformations with high efficiency and specificity. Research supported includes the molecular characterization of metabolic pathways and the signaling pathways that enhance or limit their activity in living systems, and structure/function studies of key biomolecular components, signal transducers, molecular machines, and special assemblies that play an important role in chemical transformations of interest in energy production, transformation, and use. This activity constitutes the fundamental understanding of complex, nanoscale chemical catalysis in living systems and provides the basis for manipulation of biological chemistry and the development of bioinspired and biomimetic systems for specific chemical transformations.

Capital equipment is provided for such items as lasers, detectors, imaging systems, spectrometers, and computational resources.

In FY 2007, increased emphasis will be placed upon understanding interactions that occur within the nanoscale range; this includes signal reception at biological surfaces and membranes, enzyme-substrate recognition, and the structure/function of molecular complexes and molecular machines that enable and control chemical transformations. An emerging area will be the development of new imaging tools and methods to examine metabolic and signaling pathways at both the physical-spatial and temporal scale. Within this funding, there is an increase for research related to the hydrogen economy ($+47,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Catalysis and Chemical Transformation** ................................ | **37,871** | **38,107** | **47,459** |

This activity supports basic research to understand the chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources; and the chemistry of the molecules used to create advanced materials. This activity seeks to develop these principles to enable rational design of catalysts.

Catalytic transformations impact virtually all of the energy missions of the Department. Catalysts are needed for all of the processes required to convert crude petroleum into a clean burning fuel. The production of virtually every chemical-based consumer product requires catalysts. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added chemicals. Environmental impacts from catalytic science can include minimizing unwanted products from production streams and transforming toxic chemicals into benign ones, such as chlorofluorocarbons into environmentally acceptable refrigerants. Research supported by this program also provides the basis and impetus for creating a broad range of new materials, such as mesoporous solids which have improved catalytic properties.

This activity is the Nation's major supporter of catalysis research, and it is the only activity that treats catalysis as a discipline integrating all aspects of homogeneous and heterogeneous catalysis research.

Capital equipment is provided for such items as ultrahigh vacuum equipment with various probes of surface structure, Fourier-transform infrared instrumentation, and high-field, solid-state Nuclear Magnetic Resonance (NMR) spectrometers.

In FY 2007, funding will continue to address recommendations of the FY 2002 BESAC-sponsored workshop that described new opportunities afforded by progress in the tools and concepts of nanoscience. The availability of new tools for preparation, characterization, and analysis and the merging of concepts drawn from homogeneous (single phase such as solution) catalysis, heterogeneous (between phases such as gas-surface) catalysis, and biocatalysts provide the potential to pioneer new approaches to catalysis design. New strategies for the rational design of selective oxidation catalysts and catalysts for the production of hydrogen from renewable feedstocks will be explored, and the control of self assembled nanoscale catalyst structures will be studied. Innovative hybrid materials that integrate biomimetic approaches with advances in catalysis will be performed and the nature of biologically directed mineralization that results in exquisite structural control will be studied. Basic research into the chemistry of inorganic, organic, and inorganic/organic hybrid porous materials with pores in the 1-30 nm range will be undertaken, nano-scale self-assembly of these systems will be studied, and the integration of functional catalytic properties into nanomaterials will be explored. The development of a new generation of fuel-forming catalysts is necessary for integration into both higher-order artificial photosynthetic assemblies and photoelectrochemical devices. Within this funding, there are increases for ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), solar energy conversion ($+3,659,000), and research related to the hydrogen economy ($+3,443,000).

| | | | |
|---|---|---|---|
| ▪ **Separations and Analyses** ........................................................ | **15,490** | **17,287** | **24,041** |

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop entirely new approaches to analysis such as chemical imaging in complex, heterogeneous environments. This activity is the Nation's most significant long-term investment in many aspects of separations and analysis, including solvent extraction, ion exchange, and mass spectrometry.

The goal of this activity is to obtain a thorough understanding of the basic chemical and physical principles involved in separations systems and analytical tools so that their utility can be realized.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

Work is closely coupled to the Department's stewardship responsibility for transuranic chemistry; therefore, separation and analysis of transuranic isotopes and their radioactive decay products are important components of the portfolio.

Knowledge of molecular level processes is required to characterize and treat extremely complex radioactive mixtures and to understand and predict the fate of associated contaminants in the environment. Though the cold war legacy is the most obvious of the Department's missions, the economic importance of separation science and technology is huge. For example, distillation processes in the petroleum, chemical, and natural gas industries annually consume the equivalent of 315 million barrels of oil. It has been estimated that separation processes account for more than five percent of the total national energy consumption. Separations are essential to nearly all operations in the processing industries and are also necessary for many analytical procedures. An analysis is an essential component of every chemical process from manufacture through safety and risk assessment and environmental protection.

Capital equipment is provided for such items as computational workstations and inductively coupled plasma torch spectrometers for atomic emission determination.

In FY 2007, funding will include studies at the nanoscale as well as the formation of macroscopic separation systems via self-assembly of nanoscale precursors. This work will build on recent advances in imaging single-molecule interactions and reactions and will expand our knowledge of how molecules interact with pore walls, with one another, and with other molecules to effect separation between molecules. Chemical analysis research will emphasize: (1) the study of hydrogen-separation materials and processes under realistic environmental conditions, rather than in high vacuum; (2) achievement of high temporal resolution, so that changes can be monitored dynamically; and (3) will allow multiple analytical measurements to be made simultaneously on systems such as fuel cell membranes, which have three percolation networks (proton, electron, and gas). The optimization of the light-harvesting properties of molecules on surfaces and at interfaces requires pushing the analytical means to image these molecules with the requisite spatial and temporal resolution. Within this funding, there are increases for molecular science for advanced chemical separations ($+1,000,000), chemical imaging ($+1,750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), research related to the hydrogen economy ($+808,000), and solar energy conversion ($+1,696,000).

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Heavy Element Chemistry** ....................................................... | **10,506** | **9,354** | **17,128** |

This activity supports research in actinide and fission product chemistry. Areas of interest are synthesis of actinide-containing materials; theoretical methods for, and calculation of, heavy element electronic properties, molecular structure and reactivity; aqueous and non-aqueous coordination chemistry; solution and solid-state bonding and reactivity; measurement of actinide chemical and physical properties; determination of chemical properties of the heaviest actinide and transactinide elements; and studies of the bonding relationship between the actinides, lanthanides, and transition metals.

The heavy element chemistry program, with its genesis in the Manhattan project, has explored the chemical properties of the transuranium and transactinide elements, the latter using techniques

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

developed for isotopes that have half-lives on the order of seconds to tens of seconds. In recent years the emphasis of the program returned to the chemistry of the lighter transuranium elements and fission products, driven by the necessity to characterize long-lived species found in storage at DOE production sites. Knowledge of the chemical characteristics of actinide and fission products materials under waste tank conditions is necessary to treat these complex mixtures. Accidental release of actinide and fission product materials to the environment also requires molecular bonding information in order to predict and mitigate their transport under environmental conditions. This activity is closely coupled to the BES separations and analysis activity.

This activity represents the Nation's only funding for basic research in the chemical and physical principles governing actinide and fission product chemistry. The program is primarily at the national laboratories because of the special licenses and facilities needed to obtain and safely handle substantial amounts of radioactive materials. However, research in heavy element chemistry is supported at universities, and collaborations between university and laboratory programs are encouraged. The education of graduate students and postdoctoral researchers is an important responsibility of this activity. Approximately twenty undergraduate students chosen from universities and colleges throughout the U.S. are given introductory lectures in actinide and radiochemistry each summer.

Capital equipment is provided for items used to characterize actinide materials (spectrometers, ion chambers, calorimeters, etc.) and equipment to handle the actinides safely at synchrotron light source experiments.

In FY 2007, funding will continue to include experiment, theory, and modeling to understand the chemical bonding in the heavy elements. Experimental studies will include aqueous and non-aqueous high-pressure chemistry and surface chemistry of these elements. Such studies are essential for the optimization of advanced fuel cycles for future nuclear energy needs. In addition, new beamlines at synchrotron light sources capable of handling samples of these heavy elements will permit detailed spectroscopic studies of specimens under a variety of conditions. The study of the bonding in these heavy elements may also provide new insights into organometallic chemistry, beyond that learned from "standard" organometallic chemistry based on transition metals with d-orbital bonding. Within this funding, there is an increase for mid-scale instrumentation ($+500,000) and research related to advanced fuel cycles ($+7,274,000).

- **Geosciences Research** ................................................................ **22,212** **20,494** **22,345**

The Geosciences activity supports long-term basic research in geochemistry and geophysics. Geochemical research focuses on new paradigms for aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. It seeks fundamental understanding of geochemical processes and reaction rates. Geophysical research focuses on new approaches to understand subsurface physical properties of fluids, rocks, and minerals, and how to determine them from the surface. It seeks fundamental understanding of the physics of wave propagation in complex media. This activity has pioneered the application of x-ray and neutron scattering to geochemical and geophysical studies.

Capital equipment is provided for such items as x-ray and neutron scattering end stations at the BES facilities for environmental samples, and for experimental, field, and computational capabilities.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

In FY 2007, funding will continue to provide the majority of individual investigator basic research funding for the federal government in areas with the greatest impact on unique DOE missions such as low-temperature, low-pressure geochemical processes in the subsurface. This activity provides the basic research component in solid Earth sciences to the DOE's energy resources and environmental quality portfolios. Within this funding, there are increases for nanoscale geochemistry ($+851,000), chemical imaging ($+500,000) and mid-scale instrumentation ($+500,000).

| | | | |
|---|---|---|---|
| ▪ **Chemical Energy and Chemical Engineering** | **11,938** | **3,731** | **1,817** |

This activity supports research on electrochemistry, thermophysical and thermochemical properties, and physical and chemical rate processes. Also included is fundamental research in areas critical to understanding the underlying limitations in the performance of electrochemical energy storage and conversion systems including anode, cathode, and electrolyte systems and their interactions with emphasis on improvements in performance and lifetime. The program covers a broad spectrum of research including fundamental studies of composite electrode structures; failure and degradation of active electrode materials; thin film electrodes, electrolytes, and interfaces; and experimental and theoretical aspects of phase equilibria, especially of mixtures, including supercritical phenomena.

Capital equipment is provided for such items as computer work stations and electrochemical apparatus.

In FY 2007, in order to emphasize other priorities, there will be reductions in research in the areas of physical properties related to process engineering, engineering approaches to electrochemical fuel cells, and aspects of advanced battery research.

| | | | |
|---|---|---|---|
| ▪ **General Plant Projects (GPP)** | **9,832** | **13,124** | **13,408** |

GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems principally at the Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the BES stewardship responsibilities for these laboratories. Funding of this type is essential for maintaining the productivity and usefulness of the Department-owned facilities and in meeting requirements for safe and reliable facilities operation. Additional GPP funding is included in the Facilities Operations justification in both the Materials Sciences and Engineering subprogram and the Chemical Sciences, Geosciences, and Biosciences subprogram. The total estimated cost of each GPP project will not exceed $5,000,000.

| | | | |
|---|---|---|---|
| ▪ **General Purpose Equipment (GPE)** | **4,993** | **4,017** | **4,058** |

GPE funding is provided for Ames Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory as part of the BES stewardship responsibilities for these laboratories for GPE that supports multipurpose research. Infrastructure funding is requested to maintain, modernize, and upgrade the ORNL, ANL, and Ames sites and facilities to correct deficiencies due to aging, changing technology, and inadequate past investments.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Facility Operations** | **6,437** | **6,251** | **6,805** |

The facility operations budget request, which includes operating funds, capital equipment, and GPP, is described in a consolidated manner later in this budget. This subprogram funds the Combustion Research Facility. GPP funding is also required for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems. The total estimated cost of each GPP project will not exceed $5,000,000.

## Facilities

| | | | |
|---|---|---|---|
| Combustion Research Facility | 6,437 | 6,251 | 6,805 |
| **SBIR/STTR** | **—** | **5,468** | **6,581** |

In FY 2005 $5,213,000 and $626,000 were transferred to the SBIR and STTR programs, respectively. The FY 2006 and FY 2007 amounts shown are the estimated requirements for the continuation of the SBIR and STTR program.

| | | | |
|---|---|---|---|
| **Total, Chemical Sciences, Geosciences, and Energy Biosciences** | **232,365** | **220,550** | **268,499** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Chemical Sciences, Geosciences, and Energy Biosciences Research** | |
| ▪ **Atomic, Molecular, and Optical (AMO) Science** | |
| Increases are provided for coherent control of quantum systems ($+851,000), ultrafast science ($+2,000,000), chemical imaging ($+500,000), and mid-scale instrumentation ($+500,000) | +3,851 |
| ▪ **Chemical Physics Research** | |
| Increases are provided for condensed phase and interfacial molecular science ($+1,000,000), ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), and solar energy conversion ($+1,697,000). | +5,947 |
| ▪ **Photochemistry and Radiation Research** | |
| Increases are provided for research related to the hydrogen economy ($+1,609,000), ultrafast science ($+1,000,000), and solar energy conversion ($+3,909,000) | +6,518 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Molecular Mechanisms of Natural Solar Energy Conversion** | |
| Increases are provided for biophysical characterization of biomolecular complexes ($+500,000), research related to the hydrogen economy ($+118,000), chemical imaging ($+750,000), emergent behavior ($+500,000), and solar energy conversion ($+3,909,000). | +5,777 |
| ▪ **Metabolic Regulation of Energy Production** | |
| Increase is provided for research related to the hydrogen economy | +47 |
| ▪ **Catalysis and Chemical Transformation** | |
| Increases are provided for research related to the hydrogen economy ($+3,443,000), ultrafast science ($+1,000,000), chemical imaging ($+750,000), mid-scale instrumentation ($+500,000), and solar energy conversion ($+3,659,000) | +9,352 |
| ▪ **Separations and Analyses** | |
| Increases are provided for molecular science for advanced chemical separation ($+1,000,000), research related to the hydrogen economy ($+808,000), chemical imaging ($+1,750,000), mid-scale instrumentation ($+500,000), emergent behavior ($+1,000,000), and solar energy conversion ($+1,696,000). | +6,754 |
| ▪ **Heavy Element Chemistry** | |
| Increases are provided for mid-scale instrumentation ($+500,000) and research relevant to advanced fuel cycles ($+7,274,000) | +7,774 |
| ▪ **Geosciences Research** | |
| Increases are provided for nanoscale geochemistry ($+851,000), chemical imaging ($+500,000), and mid-scale instrumentation ($+500,000) | +1,851 |
| ▪ **Chemical Energy and Chemical Engineering** | |
| Reductions in research in the areas of physical properties related to process engineering, engineering approaches to electrochemical fuel cells, and aspects of advanced battery research | -1,914 |
| ▪ **General Plant Projects (GPP)** | |
| Increase in general plant projects intended to help alleviate recurring maintenance costs by improving infrastructure. | +284 |
| ▪ **General Purpose Equipment (GPE)** | |
| Small increase for GPE maintenance of equipment | +41 |
| **Total, Chemical Sciences, Geosciences and Energy Biosciences Research** | **+46,282** |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Facility Operations** | |
| Increase for the Combustion Research Facility to support operations | +554 |
| **SBIR/STTR** | |
| Increase in SBIR/STTR funding because of an increase in operating expenses. | +1,113 |
| **Total Funding Change, Chemical Sciences, Geosciences, and Energy Biosciences** | **+47,949** |

# Construction

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Construction | | | |
| Spallation Neutron Source (ORNL) | 79,891 | 41,327 | — |
| Project Engineering Design, Nanoscale Science Research Centers | 1,996 | — | — |
| Project Engineering Design, Linac Coherent Light Source (SLAC) | 19,914 | 2,518 | 161 |
| Linac Coherent Light Source (SLAC) | 29,760 | 82,170 | 105,740 |
| Center for Functional Nanomaterials (BNL) | 18,317 | 36,187 | 18,864 |
| The Molecular Foundry (LBNL) | 31,828 | 9,510 | 257 |
| Center for Nanophase Materials Science (ORNL) | 17,669 | — | — |
| Center for Integrated Nanotechnologies (SNL/LANL) | 30,650 | 4,580 | 247 |
| Project Engineering Design, National Synchrotron Light Source-II (BNL) | — | — | 20,000 |
| Project Engineering Design, Advanced Light Source User Support Building (LBNL) | — | — | 3,000 |
| Total, Construction | 230,025 | 176,292 | 148,269 |

### Description

Construction is needed to support the research in each of the subprograms in the BES program. Experiments necessary in support of basic research require that state-of-the-art facilities be built or existing facilities modified to meet unique research requirements. Reactors, x-ray light sources, and neutron sources are among the expensive, but necessary, facilities required. The budget for the BES program includes funding for the construction and modification of these facilities.

### Benefits

The new facilities that are under construction—the Linac Coherent Light Source, the Center for Functional Nanomaterials, design of the National Synchrotron Light Source-II—continue the tradition of BES and SC of providing the most advanced scientific user facilities for the Nation's research community in the most cost effective way. All of the BES construction projects are conceived and planned with the broad user community and, during construction, are maintained on schedule and within cost. Furthermore, the construction projects all adhere to the highest standards of safety. As described in the Benefits section for the User Facilities, these facilities will provide the Nation's research community with the tools to fabricate, characterize, and develop new materials and chemical processes in order to advance basic and applied research across the full range of scientific and technological endeavor, including chemistry, physics, earth science, materials science, environmental science, biology, and biomedical science.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Spallation Neutron Source (SNS), ORNL** | **79,891** | **41,327** | **—** |

The purpose of the SNS Project is to provide a next-generation short-pulse spallation neutron source for neutron scattering. The SNS will be used by researchers from academia, national and federal labs, and industry for basic and applied research and for technology development in the fields of condensed matter physics, materials sciences, magnetic materials, polymers and complex fluids, chemistry, biology, earth sciences, and engineering. When commissioning is complete, the SNS will be significantly more powerful (by about a factor of 10) than the best spallation neutron source now in existence. The facility will be used by 1,000–2,000 scientists and engineers annually. Interest in the scientific community in the SNS is increasing.

The SNS consists of a linac-ring accelerator system that delivers short (microsecond) proton pulses to a target/moderator system where neutrons are produced by a process called spallation. The neutrons so produced are then used for neutron scattering experiments. Specially designed scientific instruments use these pulsed neutron beams for a wide variety of investigations. There will initially be one partially instrumented target station with the potential for adding more instruments and a second target station later.

The SNS project partnership among six DOE laboratories has taken advantage of specialized technical capabilities within the laboratories: Lawrence Berkeley National Laboratory in ion sources; Los Alamos National Laboratory in linear accelerators; Thomas Jefferson National Accelerator Facility in superconducting linear accelerators; Brookhaven National Laboratory in proton storage rings; Argonne National Laboratory in instruments; and Oak Ridge National Laboratory in targets and moderators.

In FY 2001, two grants were awarded to universities for research requiring the design, fabrication, and installation of instruments for neutron scattering. These instruments will be sited at the SNS, with commissioning beginning late in FY 2006, shortly after the SNS facility itself is commissioned. Both awards were made based on competitive peer review conducted under 10 CFR Part 605, Financial Assistance Program.

Funds appropriated in FY 2002 continued R&D, design, procurement, construction activities, and component installation. Essentially all R&D supporting construction of the SNS was completed, with instrument R&D continuing. Title II design was completed on the linac and was continued on the ring, target, and instrument systems. The completed ion source and portions of the drift tube linac were delivered to the site and their installation was begun. Other system components for the accelerator, ring, target, and instruments continued to be manufactured. Work on conventional facilities continued, with some reaching completion and being turned over for equipment installation, such as the ion source building and portions of the klystron building and linac tunnel. Construction work began on the ring tunnel.

Funds appropriated in FY 2003 continued instrument R&D and design, procurement, construction, installation, and commissioning. The ion source was commissioned; the drift tube linac was installed and commissioning was begun; installation of other linac components progressed; and installation of ring components began. Target building construction and equipment installation continued.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

Numerous conventional facilities, including the klystron, central utilities, and ring service buildings and the linac and ring tunnels, were advanced. Site utilities became available to support linac commissioning. In FY 2003, a Major Item of Equipment (MIE) was initiated for five SNS instruments: High-Pressure Diffractometer, High-Resolution Chopper Spectrometer, Single-Crystal Diffractometer, Disordered Materials Diffractometer, and Hybrid Polarized Beam Spectrometer. The MIE is funded at $3,143,000 in FY 2005, $12,579,000 in FY 2006, and $10,500,000 in FY 2007. These instruments will be built by individual DOE laboratories or consortia of DOE laboratories in collaboration with the SNS based on scientific merit and importance to users from universities, industries, and government laboratories. A second Major Item of Equipment is initiated in FY 2007 for an additional four to five instruments.

Funds appropriated in 2004 continued instrument R&D, design, and procurement. The drift-tube linac and cavity-coupled linac portions of the warm linac commissioning were completed. Other commissioning activities continued in the linac. Cryogenic refrigerator installation and system cool down were advanced. High-energy beam transport installation and testing were completed. Ring fabrication and assembly activities continued. Target fabrication and assembly activities continued. Most SNS buildings are completed with the exception of ongoing construction work in the target and instrument facilities and the central laboratory and office building.

Funds appropriated in FY 2005 continued R&D, procurement, and installation of equipment for instrument systems. Commissioning of Linac Systems was completed. Commissioning of the high-energy beam transport and accumulator ring was begun; installation and testing for the ring-target beam transport system was performed. Installation and testing was performed and preparation for the readiness review was started for target systems. The remaining major construction contracts were completed. Procurement, installation, and testing continued for integrated control systems.

Funds appropriated in FY 2006 will complete the SNS Project. Procurement and installation of equipment for instrument systems will be performed. An accelerator readiness review will be completed and target systems will be commissioned. All requirements to begin operations will be met and all SNS facilities will be turned over to operations. The estimated Total Project Cost is $1,411,282,560, and the construction schedule continues to call for project completion by mid-2006.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Project Engineering and Design, Nanoscale Science Research Centers** ........ | **1,996** | **—** | **—** |

Project Engineering and Design funds provide Title I and Title II design-only funding for Nanoscale Science Research Centers (NSRCs) at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, Sandia National Laboratories (Albuquerque), and Brookhaven National Laboratory. These funds were used to assure project feasibility, define the scope, and provide estimates of construction costs and schedules. NSRCs provide state-of-the-art facilities for materials nanofabrication and advanced tools for nanocharacterization to the scientific community.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Project Engineering and Design, Linac Coherent Light Source, SLAC** ........ | **19,914** | **2,518** | **161** |

The purpose of the Linac Coherent Light Source (LCLS) Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source. This advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons have revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project would provide the world's first demonstration of an x-ray free-electron-laser (FEL) in the 1.5–15 Å range.

For many years, the Basic Energy Sciences Advisory Committee (BESAC) has been actively involved with the development of such a next-generation light source. In 1997, the BESAC report "DOE Synchrotron Radiation Sources and Science" recommended funding an R&D program in next-generation light sources. In 1999, the BESAC report "Novel, Coherent Light Sources" concluded, "Given currently available knowledge and limited funding resources, the hard x-ray region (8-20 keV or higher) is identified as the most exciting potential area for innovative science. DOE should pursue the development of coherent light source technology in the hard x-ray region as a priority. This technology will most likely take the form of a linac-based free electron laser using self-amplified stimulated emission or some form of seeded stimulated emission…"

The proposed LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons; the light is coherent or "laser like" enabling many new types of experiments; and the pulses are short (230 femtoseconds with planned improvements that will further reduce the pulse length to subfemtosecond levels) enabling studies of fast chemical and physical processes. The LCLS has considerable potential as a tool for groundbreaking research in the physical and life sciences. LCLS x-rays can be used to create and observe extreme conditions in matter, such as exotic excited states of atoms and warm dense plasmas, previously inaccessible to study. They can be used to directly observe changes in molecular and material structure on the natural time scales of atomic and molecular motions. LCLS x-rays offer an opportunity to image non-periodic molecular structures, such as single or small clusters of biomolecules or nanosctructured materials, at atomic or near-atomic resolution. These are only a few examples of breakthrough science that will be enabled by LCLS, planned to be the world's first "fourth generation" x-ray light source.

The LCLS project leverages capital investments in the existing SLAC linac as well as technologies developed for linear colliders and for the production of intense electron beams with radio-frequency photocathode guns. The SLAC linac will provide high-current, low-emittance 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through a newly constructed long undulator, the electron bunches will lead to self-amplification of the emitted x-ray radiation, constituting the x-ray FEL. The availability of the SLAC linac for the LCLS Project creates a unique opportunity (worldwide) for demonstration and use of x-ray FEL radiation.

The proposed LCLS Project requires a 150 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120 meter undulator and associated equipment.

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

Funds were appropriated in FY 2006 and are requested in FY 2007 for Project Engineering Design (PED) Title I and Title II design work. Additional information on the LCLS Project is provided in the LCLS PED data sheet, project number 03-SC-002.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Linac Coherent Light Source, SLAC** ...................................... | **29,760** | **82,170** | **105,740** |

Funds appropriated in FY 2005 were used to initiate long-lead procurements. Early acquisition of selected critical path items supported pivotal schedule and technical aspects of the project. These include acquisition of the 120 MeV injector linac, acquisition of the undulator modules and the measurement system needed for verification of undulator performance, and acquisition of main linac magnets and radiofrequency (RF) systems required to produce electron beams meeting the stringent requirements of the LCLS free-electron laser.

Funds appropriated in FY 2006 will support physical construction of the LCLS conventional facilities including ground-breaking for the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and the Central Laboratory and Office Building. In addition, the injector will be completed and construction of the downstream linac and electron beam transport to the undulator hall will begin. Undulator module assembly will be started along with construction of x-ray transport/optics/diagnostics systems.

FY 2007 budget authority is requested to continue physical construction of the LCLS conventional facilities including ground-breaking for the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and the Central Laboratory and Office (CLO) building.

Performance will be measured by meeting the cost and timetables within 10% of the baseline within the construction project data sheet. Additional information on the LCLS Project is provided in the LCLS construction data sheet, project number 05-R-320.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, BNL**............................................... | **18,317** | **36,187** | **18,864** |

The Center for Functional Nanomaterials (CFN), a BES Nanoscale Science Research Center, will have as its focus understanding the chemical and physical response of nanomaterials to make functional materials such as sensors, activators, and energy-conversion devices. The facility will use existing facilities such as the NSLS and the Laser Electron Accelerator facility. It will also provide clean rooms, general laboratories, and wet and dry laboratories for sample preparation, fabrication, and analysis. Equipment will include that needed for laboratory and fabrication facilities for e-beam lithography, transmission electron microscopy, scanning probes and surface characterization, material synthesis and fabrication, and spectroscopy.

FY 2005 funding was appropriated for the start of construction, FY 2006 funding continued construction and equipment procurement, and FY 2007 funding is requested to complete construction of the Center for Functional Nanomaterials at Brookhaven National Laboratory. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 05-R-321.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL** | **31,828** | **9,510** | **257** |

The Molecular Foundry, a BES Nanoscale Science Research Center, will focus its research on the interface between soft materials such as those found in living systems and hard materials such as carbon nanotubes, and the integration of these materials into complex functional assemblies. The Molecular Foundry will use existing facilities such as the ALS, the NCEM, and the National Energy Research Scientific Computing Center. The Molecular Foundry will provide laboratories for materials science, physics, chemistry, biology, and molecular biology. State-of-the-art equipment will include clean rooms; controlled environmental rooms; scanning tunneling microscopes; atomic force microscopes; a transmission electron microscope; fluorescence microscopes; mass spectrometers; a DNA synthesizer and sequencer; a nuclear magnetic resonance spectrometer; ultrahigh vacuum scanning-probe microscopes; photo, uv, and e-beam lithography equipment; a peptide synthesizer; advanced preparative and analytical chromatographic equipment; and cell culture facilities.

FY 2004 funding was appropriated for the start of construction, FY 2005 and FY 2006 funding continued construction and equipment procurement, and FY 2007 funding will complete construction. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 04-R-313.

| | | | |
|---|---|---|---|
| ▪ **Nanoscale Science Research Center – The Center for Nanophase Materials Sciences, ORNL** | **17,669** | **—** | **—** |

The Center for Nanophase Materials Sciences (CNMS), a BES Nanoscale Science Research Center, will include a research center and user facility that will integrate nanoscale science research with neutron science, synthesis science, and theory/modeling/simulation. A new building will provide state-of-the-art clean rooms, general laboratories, and wet and dry laboratories for sample preparation, fabrication, and analysis. Included will be equipment to synthesize, manipulate, and characterize nanoscale materials and structures. The Center, collocated at the Spallation Neutron Source complex, will have as its major scientific thrusts nano-dimensioned soft materials, complex nanophase materials systems, and the crosscutting areas of interfaces and reduced dimensionality that become scientifically critical on the nanoscale. A major focus of the CNMS will be to exploit ORNL's unique facilities and capabilities in neutron scattering.

FY 2004 and FY 2005 funding was requested for the construction of the Center for Nanophase Materials Science located at Oak Ridge National Laboratory. Performance was measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet.

| | | | |
|---|---|---|---|
| ▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, SNL/LANL** | **30,650** | **4,580** | **247** |

The Center for Integrated Nanotechnologies (CINT), a BES Nanoscale Science Research Center, will focus on exploring the path from scientific discovery to the integration of nanostructures into the micro- and macro-worlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

nanoscale materials and structures. CINT focus areas are nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nanoscale/bio/microscale interfaces. CINT will be jointly administered by Los Alamos National Laboratory and Sandia National Laboratories. This Center will make use of a wide range of specialized facilities including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory at LANL.

FY 2003 funding was appropriated for the start of construction, FY 2004, FY 2005, and FY 2006 funding continued construction and equipment procurement, and FY 2007 funding will complete construction for the Center for Integrated Nanotechnologies managed jointly by Sandia National Laboratories and Los Alamos National Laboratory. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 03-R-313.

| | | | |
|---|---|---|---|
| ▪ **Project Engineering and Design, National Synchrotron Light Source-II (NSLS-II), BNL** | **—** | **—** | **20,000** |

The NSLS-II would be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of one nanometer (nm), an energy resolution of 0.1 millielectron volt (meV), and the ultra-high sensitivity required to perform spectroscopy on a single atom. NSLS-II will be the best storage-ring-based synchrotron light source in the world, but, more importantly, NSLS-II will be transformational in that it will open new regimes of scientific discovery and investigation.

FY 2007 funding is requested to begin Project Engineering and Design (PED) Title I and Title II design. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 07-SC-06.

| | | | |
|---|---|---|---|
| ▪ **Project Engineering and Design, Advanced Light Source (ALS) User Support Building, LBNL** | **—** | **—** | **3,000** |

The ALS User Support Building will provide high-quality user support space in sufficient quantity to accommodate the very rapid growth in the number of ALS users and to accommodate projected future expansion. The User Support Building will provide staging areas for ALS experiments, space for a long beamline that will extend from the floor of the ALS into the User Support Building, and temporary office space for visiting users. FY 2007 funding is requested to begin Project Engineering and Design. Performance will be measured by meeting the cost and timetables within 10% of the baseline in the construction project data sheet. Additional information is provided in the construction project data sheet 07-SC-12.

| | | | |
|---|---|---|---|
| **Total, Construction** | **230,025** | **176,292** | **148,269** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ **Spallation Neutron Source, ORNL** | |
| Decrease in funding for construction of the Spallation Neutron Source at ORNL, representing the scheduled completion of the project................................................ | -41,327 |
| ▪ **Project Engineering and Design, Linac Coherent Light Source** | |
| Decrease in funding for Project Engineering and Design (PED) related to design-only activities for the Linac Coherent Light Source (LCLS) at SLAC, representing the scheduled decrease in activities. ........................................................................... | -2,357 |
| ▪ **Linac Coherent Light Source, SLAC** | |
| Increase in funding to continue construction for the LCLS project............................ | +23,570 |
| ▪ **Nanoscale Science Research Center – The Center for Functional Nanomaterials, BNL** | |
| Decrease in funding for construction of the Center for Functional Nanomaterials at BNL, representing the scheduled ramp down of activities........................................ | -17,323 |
| ▪ **Nanoscale Science Research Center – The Molecular Foundry, LBNL** | |
| Decrease in funding for construction of the Molecular Foundry at LBNL, representing the scheduled ramp down of activities.................................................. | -9,253 |
| ▪ **Nanoscale Science Research Center – The Center for Integrated Nanotechnologies, SNL/LANL** | |
| Decrease in funding for construction of the Center for Integrated Nanotechnologies at SNL/LANL, representing the scheduled ramp down of activities......................... | -4,333 |
| ▪ **Project Engineering and Design, National Synchrotron Light Source-II (NSLS II), BNL** | |
| Increase in funding to initiate Project Engineering and Design ................................ | +20,000 |
| ▪ **Project Engineering and Design, Advanced Light Source (ALS) User Support Building, LBNL** | |
| Increase in funding to initiate Project Engineering and Design ................................ | +3,000 |
| **Total Funding Change, Construction**............................................................................ | **-28,023** |

# Major User Facilities

## Funding Schedule by Activity

Funding for the operation of these facilities is provided in the Materials Sciences and Engineering, and the Chemical Sciences, Geosciences, and Energy Biosciences subprograms.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Major User Facilities | | | |
| Advanced Light Source at Lawrence Berkeley National Laboratory. | 44,800 | 42,783 | 49,802 |
| Advanced Photon Source at Argonne National Laboratory | 100,500 | 95,890 | 108,604 |
| National Synchrotron Light Source at Brookhaven National Laboratory | 36,750 | 36,196 | 40,763 |
| Center for Nanophase Materials Sciences at Oak Ridge National Laboratory | — | 17,800 | 19,190 |
| Center for Integrated Nanotechnologies at Sandia National Laboratories/Albuquerque and Los Alamos National Laboratory | — | 11,900 | 19,190 |
| Molecular Foundry at Lawrence Berkeley National Laboratory | — | 8,100 | 19,190 |
| Center for Nanoscale Materials at Argonne National Laboratory | — | 3,500 | 19,190 |
| Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center. | 32,388 | 25,475 | 35,836 |
| High Flux Isotope Reactor at Oak Ridge National Laboratory. | 46,900 | 43,330 | 51,598 |
| Radiochemical Engineering Development Center (REDC) at Oak Ridge National Laboratory. | 4,500 | — | — |
| Intense Pulsed Neutron Source at Argonne National Laboratory. | 16,800 | 15,500 | 18,531 |
| Manuel Lujan, Jr. Neutron Scattering Center at Los Alamos National Laboratory. | 9,588 | 10,000 | 10,582 |
| Spallation Neutron Source at Oak Ridge National Laboratory. | 37,600 | 101,001 | 171,409 |
| Combustion Research Facility at Sandia National Laboratories/California. | 6,437 | 6,251 | 6,805 |
| National Synchrotron Light Source-II at Brookhaven National Laboratory | 1,000 | — | 25,000 |
| Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center | — | 3,500 | 16,000 |
| Linac for LCLS | — | 29,700 | 40,000 |
| Total, Major User Facilities | 337,263 | 450,926 | 651,690 |

### Description

The BES scientific user facilities provide experimental capabilities that are beyond the scope of those found in laboratories of individual investigators. Synchrotron radiation light sources, high-flux neutron sources, electron beam microcharacterization centers, and other specialized facilities enable scientists to carry out experiments that could not be done elsewhere. These facilities are part of the Department's system of scientific user facilities, the largest of its kind in the world.

# Capital Operating Expenses and Construction Summary

## Capital Operating Expenses

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| General Plant Projects | 16,532 | 13,695 | 15,624 |
| Accelerator Improvement Projects | 10,245 | 8,032 | 25,112 |
| Capital Equipment | 86,639 | 69,123 | 131,657 |
| Total, Capital Operating Expenses | 113,416 | 90,850 | 172,393 |

## Construction Projects

(dollars in thousands)

| | Total Estimated Cost (TEC) | Prior Year Appro-priations | FY 2005 | FY 2006 | FY 2007 | Unappro-priated Balances |
|---|---|---|---|---|---|---|
| 07-SC-06, PED, BNL, National Synchrotron Light Source-II | 75,000 | — | — | — | 20,000 | 55,000 |
| 07-SC-12, PED, LBNL, Advanced Light Source User Support Building | 3,000 | — | — | — | 3,000 | — |
| 05-R-320, SLAC, Linac Coherent Light Source | 315,000[a] | — | 29,760 | 82,170 | 105,740 | 61,356 |
| 05-R-321, BNL, Center for Functional Nanomaterials | 79,700[b] | — | 18,317 | 36,187 | 18,864 | 366 |
| 04-R-313, LBNL, The Molecular Foundry | 83,604[c] | 34,794 | 31,828 | 9,510 | 257 | — |
| 03-SC-002, PED, SLAC, Linac Coherent Light Source | 35,974 | 13,381 | 19,914 | 2,518 | 161 | — |
| 03-R-312, ORNL, Center for Nanophase Materials Sciences | 63,740[d] | 43,583 | 17,669 | — | — | — |
| 03-R-313, SNL, Center for Integrated Nanotechnologies | 73,754[e] | 34,118 | 30,650 | 4,580 | 247 | — |
| 02-SC-002 PED, Nanoscale Science Research Centers | 19,828 | 17,832 | 1,996 | — | — | — |
| 99-E-334, ORNL, Spallation Neutron Source | 1,192,283 | 1,071,065 | 79,891 | 41,327 | — | — |
| Total, Construction | | | 230,025 | 176,292 | 148,269 | |

[a] Includes $35,974,000 of PED included in the 03-SC-002 PED, SLAC, Linac Coherent Light Source datasheet.
[b] Includes $5,966,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[c] Includes $7,215,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[d] Includes $2,488,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.
[e] Includes $4,159,000 of PED included in the 02-SC-002 PED, Nanoscale Science Research Centers datasheet.

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

(dollars in thousands)

| | Total Project Cost (TPC) | Total Estimated Cost (TEC) | Prior Year Appro-priations | FY 2005 | FY 2006 | FY 2007 | Completion Date |
|---|---|---|---|---|---|---|---|
| ANL, Center for Nanoscale Materials....... | 72,500[a] | 36,000 | 10,000 | 12,000 | 14,000 | — | FY 2006 |
| ORNL, Spallation Neutron Source Instrumentation I[b] .......... | 68,500 | 68,500 | 13,022 | 3,143 | 12,579 | 10,500 | FY 2007–FY 2011 est. |
| LBNL, Transmission Electron Aberration Corrected Microscope.... | 25,000–30,000 | 11,200–13,500 | — | — | 2,000 | 3,500 | TBD |
| ORNL, Spallation Neutron Source Instrumentation II .......... | 40,000–60,000 | 40,000–60,000 | — | — | — | 10,000 | TBD |
| SLAC, Linac Coherent Light Source Instumentation ............... | 50,000–60,000 | 50,000–60,000 | — | — | — | 10,000 | TBD |
| Total, Major Items of Equipment ................. | | | 23,022 | 15,143 | 28,579 | 34,000 | |

[a] This includes $36,000,000 provided by the State of Illinois for construction of the building.
[b] This FY 2003 MIE includes five instruments: High-Pressure Diffractometer, High-Resolution Chopper Spectrometer, Single-Crystal Diffractometer, Disordered Materials Diffractometer, and Hybrid Polarized Beam Spectrometer.

# 07-SC-06, Project Engineering and Design (PED),
# National Synchrotron Light Source II, Brookhaven National Laboratory

## 1. Significant Changes

This is the initial project engineering and design datasheet for this project.

## 2. Design, Construction, and D&D Schedule

(fiscal quarter)

| | Preliminary Design start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2007 ....... | 2Q FY 2007 | 4Q FY 2008 | N/A | N/A | N/A | N/A |

## 3. Baseline and Validation Status[a]

(dollars in thousands)

| | TEC | OPC, except D&D Costs | Offsetting D&D Costs | Total Project Costs | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2007 ............. | 75,000 | 46,000 | N/A | 121,000 | N/A | 121,000 |

## 4. Project Description, Justification, and Scope

The National Synchrotron Light Source II (NSLS-II) would be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability. It will also provide advanced insertion devices, optics, detectors, robotics, and an initial suite of scientific instruments. Together, these will enable the study of material properties and functions with a spatial resolution of ~1 nm, an energy resolution of ~0.1 meV, and the ultra-high sensitivity required to perform spectroscopy on a single atom.

Major advances in energy technologies will require scientific breakthroughs in developing new materials with advanced properties. A broad discussion is given in several recent reports, including the Basic Energy Sciences Advisory Committee Reports *Opportunities for Catalysis in the 21st Century* and *Basic Research Needs to Assure a Secure Energy Future*, the Basic Energy Sciences (BES) reports *Basic Research Needs for the Hydrogen Economy* and *Basic Research Needs for Solar Energy Utilization*, the Report of the Nanoscale Science, Engineering, and Technology Subcommittee of the National Science and Technology Committee *Nanoscience Research for Energy Needs*, and the Nuclear Energy Research Advisory Committee Report *A Technology Roadmap for Generation IV Nuclear Energy Systems*.

Collectively, these reports underscore the need to develop new tools that will allow the characterization of the atomic and electronic structure, the chemical composition, and the magnetic properties of materials *with nanoscale resolution*. Needed are non-destructive tools to image and characterize buried structures and interfaces, and these tools must operate in a wide range of temperature and harsh

[a] The estimates in section 3 are for PED only. The full project TPC (design and construction) range approved at Critical Decision-0, Approve Mission Need, excluding offsetting D&D, is $600,000,000 to $800,000,000. This estimate is preliminary and should not be construed to be validated project baseline.

environments. The absence of any tool possessing these combined capabilities was identified as a key barrier to progress in the 1999 BES Report *Nanoscale Science, Engineering and Technology Research Directions*.

In order to fill this capability gap and to further the accomplishment of its mission, the BES program will need a synchrotron light source that will enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. NSLS-II will provide these capabilities. Only x-ray methods have the potential of satisfying all of these requirements, but advances both in x-ray optics and in x-ray brightness and flux are required to achieve a spatial resolution of 1 nm and an energy resolution of 0.1 meV.

There are no alternative tools with a spatial resolution of 1 nm and energy resolution of 0.1 meV that also have the required capabilities of being non-destructive and able to image and characterize buried structures and interfaces in a wide range of temperatures and harsh environments. An analysis found that upgrading existing light sources was either impossible or not very cost effective. In the case of NSLS-I, it was found that it would be impossible to upgrade this light source due to numerous technical difficulties, including accelerator physics and infrastructure constraints, such as its small circumference, which limit the feasible in-place upgrade options.

Research and Development activities funded under Other Project Costs will address technical risk in four key areas: energy resolution, spatial resolution, superconducting undulators, and superconducting storage ring magnets.

The NSLS-II project will design, build, and install the accelerator hardware, experimental apparatus, civil construction, and central facilities required to produce a new synchrotron light source. It includes a third generation storage ring, full energy injector, experimental areas, and appropriate support equipment, all housed in a new building.

The Project Engineering and Design (PED) funds requested for NSLS-II will allow the project to proceed from conceptual design into preliminary and detailed design. These funds will assure project feasibility, define the scope, provide detailed estimates of construction costs based on the approved design, develop working drawings and specifications, and provide schedules for construction and procurements. Should a decision to proceed with construction be reached, this design effort will ensure that construction could begin on schedule in FY 2009.

The project will be conducted in accordance with the project management requirements in DOE Order 413.3 and DOE Manual 413.3-1, Program and Project Management for the Acquisition of Capital Assets. The project costs presented in this datasheet are preliminary estimates for project engineering and design only. The preliminary schedule for project Critical Decisions is as follows:

### Compliance with Project Management Order

- Critical Decision-0: Approve Mission Need—4Q FY 2005
- Critical Decision-1: Approve Preliminary Baseline Range—2Q FY 2007
- Performance Baseline External Independent Review Final Report—1Q FY 2008
- Critical Decision-2: Approve Performance Baseline—1Q FY 2008

- Critical Decision-3: Approve Start of Construction—4Q FY 2008
- Critical Decision-4: Approve Start of Operations—FY 2013

## 5. Financial Schedule (dollars in thousands)

| | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design by Fiscal Year | | | |
| 2007 | 20,000 | 20,000 | 19,000 |
| 2008 | 55,000 | 55,000 | 56,000 |
| Total, Design PED | 75,000 | 75,000 | 75,000 |

## 6. Details of Project Cost Estimate

## Total Estimated Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Preliminary and Final Design | 75,000 | N/A |

## Other Project Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Conceptual Planning | 1,000 | N/A |
| R&D | 45,000 | N/A |
| Total, OPC | 46,000 | N/A |

## 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC(Design) | — | 14,000 | 61,000 | — | — | — | — | 75,000 |
| OPC (Design) | 1,000 | 25,000 | 20,000 | — | — | — | — | 46,000 |
| Total, Project Costs (Design) | 1,000 | 39,000 | 81,000 | — | — | — | — | 121,000 |

## 8. Related Operations and Maintenance Funding Requirements

Not applicable for project engineering and design.

## (Related Funding Requirements)

Not applicable for project engineering and design.

## 9. Required D&D Information

Not applicable for project engineering and design.

## 10. Acquisition Approach (formerly Method of Performance)

A formal acquisition strategy will be prepared prior to CD-1 estimated for 1Q FY 2007.

# 07-SC-12, Project Engineering and Design (PED), Advanced Light Source User Support Building, Lawrence Berkeley National Laboratory

## 1. Significant Changes

This is the initial project engineering and design datasheet for this project.

## 2. Design, Construction, and D&D Schedule

(fiscal quarter)

| | Preliminary Design start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2007....... | 1Q FY 2007 | 2Q FY 2008 | N/A | N/A | N/A | N/A |

## 3. Baseline and Validation Status[a]

(dollars in thousands)

| | TEC | OPC, except D&D Costs | Offsetting D&D Costs | Total Project Costs | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2007 ............ | 3,000 | 400 | N/A | 3,400 | N/A | 3,400 |

## 4. Project Description, Justification, and Scope

At Lawrence Berkeley National Laboratory (LBNL), there is a critical shortage of high quality user support space. Users are presently accommodated in Building 10 and adjacent spaces that are ill-suited for their current use, and in the case of Building 10, structurally deficient. This shortage of suitable space for users creates significant impediments to the attainment of mission objectives. The User Support Building will support the major BES user facilities at LBNL, primarily the Advanced Light Source (ALS), the Office of Science's only third generation UV and soft x-ray synchrotron radiation source. The new building will also allow construction of an ultra-high resolution ALS beamline in an energy range suitable for use by multiple physical science and life science users. The unique science being performed at the ALS, cannot be supported by facilities at any other location. In particular, assembly of experimental equipment for use at the ALS needs to be performed in high-quality space located adjacent to the facility. The project is consistent with LBNL's Strategic Facilities Plan.

This project will provide a new facility of approximately 30,000 gross square foot (gsf) that includes a high bay for assembly of experimental equipment, precision component assembly areas, wet laboratories, and office space. It will be designed to support over 2,000 scientific facility users annually that are expected due to the growth of user programs at LBNL. The User Support Building project scope will also include road improvements to provide better access to the new User Support Building facility. Sustainable building principles will be incorporated into the design and construction.

The Project Engineering and Design (PED) funds requested in FY 2007 for the User Support Building will allow the project to proceed from conceptual design into preliminary and detailed design. These funds will be used to further define the scope, provide detailed estimates of construction costs based on

[a] The estimates in section 3 are for PED only. The full project TEC (design and construction) is estimated to be in the range of $30,000,000 to $35,000,000. This estimate is preliminary and should not be construed to be a validated project baseline.

the approved design, develop working drawings and specifications, and provide schedules for construction and procurements. The design effort will ensure that construction can start in FY 2008.

The project will be conducted in accordance with the project management requirements in DOE Order 413.3 and DOE Manual 413.3-1, Program and Project Management for the Acquisition of Capital Assets. The project costs represented in this datasheet are preliminary estimates for project engineering and design only. The preliminary schedule for project Critical Decisions is as follows:

**Compliance with Project Management Order**

- Critical Decision-0: Approve Mission Need—3Q FY 2003
- Critical Decision-1: Approve Preliminary Baseline Range—3Q FY 2006
- External Independent Review Final Report—1Q FY 2007
- Critical Decision-2: Approve Performance Baseline—1Q FY 2007
- Critical Decision-3: Approve Start of Construction—4Q FY 2007
- Critical Decision-4: Approve Start of Operations—FY 2010

## 5. Financial Schedule (dollars in thousands)

| | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design by Fiscal Year | | | |
| 2007 | 3,000 | 3,000 | 2,700 |
| 2008 | — | — | 300 |
| Total, Design PED | 3,000 | 3,000 | 3,000 |

## 6. Details of Project Cost Estimate

## Total Estimated Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Preliminary and Final Design | 3,000 | N/A |

## Other Project Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Conceptual Planning | 400 | N/A |

## 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC(Design)..................... | — | 2,700 | 300 | — | — | — | — | 3,000 |
| OPC (Design).................... | 400 | — | — | — | — | — | — | 400 |
| Total, Project Costs (Design) ............................ | 400 | 2,700 | 300 | — | — | — | — | 3,400 |

## 8. Related Operations and Maintenance Funding Requirements

Not applicable for project engineering and design.

## (Related Funding Requirements)

Not applicable for project engineering and design.

## 9. Required D&D Information

Not applicable for project engineering and design.

## 10. Acquisition Approach

A formal acquisition strategy will be prepared prior to CD-1 (estimated for 3Q FY 2006).

# 05-R-320, Linac Coherent Light Source,
# Stanford Linear Accelerator Center, Menlo Park, California

## 1. Significant Changes

There have been no significant changes to scope, cost, or schedule.

## 2. Design, Construction, and D&D Schedule

(fiscal quarter)

| | Preliminary Design Start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2006 ..... | 2Q FY 2003 | 4Q FY 2006 | 3Q FY 2006 | 2Q FY 2009 | N/A | N/A |
| FY 2007 ..... | 2Q FY 2003 | 4Q FY 2006 | 3Q FY 2006 | 2Q FY 2009 | N/A | N/A |

## 3. Baseline and Validation Status

(dollars in thousands)

| | TEC[a] | OPC, Except D&D Costs | Offsetting D&D Costs | Total Project Costs[a] | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2006 ..... | 315,000 | 64,000 | — | 379,000 | 379,000 | N/A |
| FY 2007 ..... | 315,000 | 64,000 | — | 379,000 | 379,000 | N/A |

## 4. Project Description, Justification, and Scope

The purpose of the Linac Coherent Light Source (LCLS) Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak brightness than any existing coherent x-ray light source. This advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project will provide the first demonstration of an x-ray Free Electron Laser (FEL) in the 1.5–15 Angstrom range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems described below. This will be the world's first such facility.

The LCLS is based on the existing SLAC linac. The SLAC linac can accelerate electrons or positrons to 50 GeV for colliding beam experiments and for nuclear and high-energy physics experiments on fixed targets. At present, the first two-thirds of the linac is being used to inject electrons and positrons into PEP-II, and the entire linac is used for fixed target experiments. When the LCLS is completed, the latter activity will be limited to 25 percent of the available beam time and the last one-third of the linac will be available for the LCLS a minimum of 75 percent of the available beam time. For the LCLS, the linac will produce high-brightness 5–15 GeV electron bunches at a 120 Hertz repetition rate. When traveling through the new 120 meter long LCLS undulator, these electron bunches will amplify the emitted x-ray radiation to produce an intense, coherent x-ray beam for scientific research.

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[a] The full project TEC and TPC, established at Critical Decision 2b (Approve Performance Baseline), are $315,000,000 and $379,000,000, respectively, and include the costs for PED from project 03-SC-002.

The LCLS makes use of technologies developed for SLAC and the next generation of linear colliders, as well as the progress in the production of intense electron beams with radiofrequency photocathode guns. These advances in the creation, compression, transport, and monitoring of bright electron beams make it possible to base this next generation of x-ray synchrotron radiation sources on linear accelerators rather than on storage rings.

The LCLS will have properties vastly exceeding those of current x-ray sources (both synchrotron radiation light sources and so-called "table-top" x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser-like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing $10^{11}$ x-ray photons in a pulse with duration of less than 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific application in the chemical, material, and biological sciences.

The LCLS Project requires a 135 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one-third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new undulator and associated equipment. Two new buildings, the Near Experimental Hall and the Far Experimental Hall, will be constructed and connected by the beam line tunnel. A Central Laboratory and Office Building will be constructed to provide laboratory and office space for LCLS users and serve as a center of excellence for basic research in x-ray physics and ultrafast science.

The combined characteristics (spectral content, peak power, pulse duration, and coherence) of the LCLS beam are far beyond those of existing light sources. The demands placed on the x-ray instrumentation and optics required for scientific experiments with the LCLS are unprecedented. The LCLS experimental program will commence with: measurements of the x-ray beam characteristics and tests of the capabilities of x-ray optics; instrumentation; and techniques required for full exploitation of the scientific potential of the facility. For this reason, the project scope includes a comprehensive suite of instrumentation for characterization of the x-ray beam and for early experiments in atomic, molecular, and optical physics. The experiments include x-ray multiphoton processes with isolated atoms, simple molecules, and clusters. Also included in the scope of the LCLS Project are the instrumentation and infrastructure necessary to support research at the LCLS, such as experiment hutches and associated interlock systems; computers for data collection and data analysis; devices for attenuation and collimation of the x-ray beam; prototype optics for manipulation of the intense x-ray beam; and synchronized pump lasers.

Beyond the scope of the LCLS construction project, an instrument development program has been implemented in order to qualify and provide instruments for the LCLS. The key element of this program is a Major Item of Equipment—the LCLS Ultrafast Science Instruments (LUSI) project. Instrument proposals will undergo a scientific peer review process to evaluate technical merit; those concepts that are accepted may then establish interface agreements with the LCLS Project. Expected funding sources include appropriated funds through the Department of Energy and other Federal agencies, private industry, and foreign entities. These instruments will all be delivered after completion of the LCLS line item project. The LCLS Scientific Advisory Committee, working in coordination with the broad scientific community, has already identified a number of high priority initial experiments that are summarized in the document, *LCLS: The First Experiments*. Five specific areas of experimentation are: fundamental studies of the interaction of intense x-ray pulses with simple atomic systems; use of LCLS to create warm dense matter and plasmas; structural studies on single nanoscale particles and biomolecules; ultrafast dynamics in chemistry and solid-state physics; and studies of nanoscale structure and dynamics in condensed matter. The combination of extreme brightness and short pulse length will make it possible to follow dynamical processes in chemistry and condensed matter physics in real time. It may also enable the determination of the structure of single biomolecules or small nanocrystals using only the diffraction pattern from a single moiety. This application has great potential in structural biology, particularly for important systems, such as membrane proteins, which are virtually uncharacterized by x-ray crystallography because they are nearly impossible to crystallize. Instrument teams will form to propose instruments to address these and other scientific areas of inquiry.

Construction funding provided in FY 2005 was for selected long-lead items, and the necessary refurbishment of existing space to provide for a magnet measurement facility for the testing of the long-lead equipment. Early acquisition of selected critical path items have supported pivotal schedule and technical aspects of the project. These include acquisition of the 135 MeV injector linac, acquisition of the undulator modules and the measurement system needed for verification of undulator performance, and acquisition of main linac magnets and radiofrequency systems required to produce electron beams meeting the stringent requirements of the LCLS FEL. Early acquisition of the 135 MeV injector was required to support initial tests of the FEL. Acquisition of the undulators in FY 2005 will enable their delivery in FY 2007. The main linac magnets and radiofrequency systems must be ready for operation shortly after the linac has reached its performance goals.

The FY 2006 funding supports physical construction of the LCLS conventional facilities including ground-breaking for the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, and the Central Laboratory and Office Building. In addition, the injector will be completed and construction of the downstream linac and electron beam transport to the undulator hall will begin. Undulator module assembly will be started along with construction of x-ray transport/optics/diagnostics systems.

Construction funding requested in FY 2007 is for continuation of physical construction of the LCLS conventional facilities including the LCLS Near Experimental Hall, Undulator Hall, Beam Transfer Hall, connecting beam transfer tunnels, Far Experimental Hall, and the Central Laboratory and Office Building. In addition, the assembly and delivery of the undulators and undulator infrastructure to SLAC's Magnetic Measurement Facility is planned, as well as the procurements for the x-ray optics, diagnostics, and end stations. Delivery of the undulators in FY 2007 enables achievement of performance goals in FY 2009.

This project will be conducted in accordance with the project management requirements in DOE Order 413.3 and DOE Manual 413.3–1, Program and Project Management for the Acquisition of Capital Assets.

**Compliance with Project Management Order:**

- Critical Decision-0: Approve Mission Need—3Q FY 2001
- Critical Decision-1: Approve Preliminary Baseline Range—1Q FY 2003
- Critical Decision-2a: Approve Long-Lead Procurement Budget—3Q FY 2003
- Critical Decision-2b: Approve Performance Baseline—3Q FY 2005
- External Independent Review Final Report—3Q FY 2005
- Critical Decision-3a: Approve Start of Long-Lead Procurement—1Q FY 2005

- Critical Decision-3b: Approve Start of Construction—2Q FY 2006
- Critical Decision-4: Approve Start of Operations—2Q FY 2009

## 5. Financial Schedule (dollars in thousands)

| | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design/Construction by Fiscal Year | | | |
| Design | | | |
| 2003 | 5,925[a] | 5,925[a] | 3,644 |
| 2004 | 7,456[a] | 7,456[a] | 9,713 |
| 2005 | 19,914[a] | 19,914[a] | 18,388 |
| 2006 | 2,518[a] | 2,518[a] | 4,056 |
| 2007 | 161[a] | 161[a] | 173 |
| Total, Design PED (03-SC-002) | 35,974 | 35,974 | 35,974 |
| | | | |
| Construction | | | |
| 2005 | 29,760[bc] | 29,760[bc] | 19,959 |
| 2006 | 82,170[c] | 82,170[c] | 87,911 |
| 2007 | 105,740[c] | 105,740[c] | 107,000 |
| 2008 | 51,356[c] | 51,356[c] | 47,856 |
| 2009 | 10,000 | 10,000 | 16,300 |
| Total, Construction | 279,026 | 279,026 | 279,026 |
| Total, TEC | 315,000 | 315,000 | 315,000 |

[a] PED funding was reduced by $75,000 as a result of the FY 2003 general reduction and rescission, by $44,000 as a result of the FY 2004 rescission, by $161,000 as a result of the FY 2005 rescission, and by $26,000 as a result of the FY 2006 rescission. This total reduction is restored in FY 2005, FY 2006, FY 2007, and FY 2008 to maintain the TEC and project scope.

[b] FY 2005 funding was for long-lead procurements. The scope of work in FY 2005 was expanded to include modification of existing facilities at the Stanford Linear Accelerator Center for testing of the long-lead equipment items.

[c] Construction funding was reduced by $240,000 as a result of the FY 2005 rescission and by $830,000 as a result of the FY 2006 rescission. This total reduction is restored in FY 2007 and FY 2008 to maintain the TEC and project scope.

## 6. Details of Project Cost Estimate

### Total Estimated Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Preliminary and Final Design (PED 03-SC-002) | 35,974 | 36,000 |
| Construction Phase | | |
| Site Preparation | 9,000 | 9,000 |
| Equipment | 110,652 | 105,800 |
| All other construction | 93,400 | 93,400 |
| Contingency | 65,974 | 70,800 |
| Total, Construction | 279,026 | 279,000 |
| Total, TEC | 315,000 | 315,000 |

### Other Project Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Conceptual Planning[a] | 7,500 | 7,500 |
| Start-up[b] | 48,383 | 51,040 |
| Contingency for OPC other than D&D | 8,117 | 5,460 |
| Total, OPC | 64,000 | 64,000 |

## 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC (Design) | 35,801 | 173 | — | — | — | — | — | 35,974 |
| TEC (Construction) | 107,870 | 107,000 | 47,856 | 16,300 | — | — | — | 279,026 |
| OPC Other than D&D | 11,000 | 16,000 | 15,500 | 21,500 | — | — | — | 64,000 |
| Total, Project Costs | 154,671 | 123,173 | 63,356 | 37,800 | — | — | — | 379,000 |

## 8. Related Operations and Maintenance Funding Requirements

| | |
|---|---|
| Start of Operation or Beneficial Occupancy (fiscal year) | 3Q FY 2009 |
| Expected Useful Life (number of years) | 30 |
| Expected Future start of D&D for new construction (fiscal year) | N/A |

[a] Costs in this category include NEPA, conceptual design, and R&D.
[b] Costs in this category include start-up (pre-operations) and spares.

## (Related Funding Requirements)

| | (dollars in thousands) | | | |
|---|---|---|---|---|
| | Annual Costs | | Life cycle costs | |
| | Current Estimate[a] | Prior Estimate | Current Estimate[b] | Prior Estimate |
| Operations | 25,000 | N/A | — | N/A |
| Maintenance | 25,000 | N/A | — | N/A |
| Total Related Funding | 50,000 | N/A | 1,909,000 | N/A |

FY 2010 is expected to be the first full year of LCLS facility operations. The current estimate is preliminary and based on historical experience with operating similar types and sizes of facilities. This estimate will be refined as the LCLS Project matures.

The estimate includes LCLS facility operations only. It does not include operation of the SLAC linac which is funded by HEP in FY 2005 and prior years, but begins a 3 to 4 year transition to BES funding beginning in FY 2006. Operation of the SLAC Linac is essential to the operation of the LCLS.

## 9. Required D&D Information

Not applicable.

## 10. Acquisition Approach

A Conceptual Design Report (CDR) for the project has been completed and reviewed. Key design activities are being specified in the areas of the injector, undulator, x-ray optics and experimental halls to reduce schedule risk to the project and expedite the startup. Also, the LCLS management systems have been put in place and tested during the Project Engineering Design (PED) phase. These activities are managed by the LCLS Project Office at SLAC, with additional portions of the project being executed by staff at Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL).

The design of technical systems is being accomplished by the three collaborating laboratories. The conventional construction design aspect (experimental halls, tunnel connecting the halls, and a Central Laboratory and Office Building) was contracted to an experienced Architect/Engineering (A/E) firm to perform Title I and II design. Title I design was completed in FY 2004. Title II design began in FY 2005.

[a] LCLS is currently under construction and normal operations are expected to begin in the 3Q FY 2009. The Annual Cost estimate shown in the table above is for a full year of operation.
[b] Assumptions: $379,000,000 TPC; $50,000,000 annual costs for 30 years; $30,000,000 de-commissioning.

## 05-R-321, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York

## 1. Significant Changes

There have been no significant changes to scope, cost, or schedule.

## 2. Design, Construction, and D&D Schedule

(fiscal quarter)

| | Preliminary Design start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2006....... | 4Q FY 2003 | 4Q FY 2004 | 3Q FY 2005 | 3Q FY 2008 | N/A | N/A |
| FY 2007....... | 4Q FY 2003 | 1Q FY 2005 | 4Q FY 2005 | 3Q FY 2008 | N/A | N/A |

## 3. Baseline and Validation Status

(dollars in thousands)

| | TEC[a] | OPC, except D&D Costs | Offsetting D&D Costs | Total Project Costs[a] | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2006 ............ | 79,700 | 1,300 | N/A | 81,000 | 81,000 | N/A |
| FY 2007 ............ | 79,700 | 1,300 | N/A | 81,000 | 81,000 | N/A |

## 4. Project Description, Justification, and Scope

This project will establish a Nanoscale Science Research Center (NSRC) at BNL. The scientific theme of the BNL Center for Functional Nanomaterials (CFN) is "atomic tailoring of functional nanomaterials to achieve a specific response." The CFN will be a user facility designed to provide a wide range of tools for the preparation and characterization of nanomaterials. The CFN will seek to integrate these unique capabilities with other BNL facilities, including the broad range of synchrotron characterization techniques available at the National Synchrotron Light Source (NSLS).

The CFN will be a new building, located across the street from the existing NSLS. Siting of the CFN will take advantage of close proximity to the Instrumentation Division and the Departments of Physics, Materials Science, and NSLS, which are key interdisciplinary participants in nanoscience research.

The design and scope of the CFN will fulfill DOE mission needs and incorporate input from potential users, gained through many channels including outreach efforts such as workshops. An essential component of the project is to establish an organizational infrastructure open to external users based on peer review. In this way a truly national nanomaterials effort can create breakthrough opportunities. The laboratory areas are organized into seven facilities established to provide the necessary primary user service. The facility theme functions cover a wide range of physical and chemical synthesis and characterization. They are designated Nanopatterning, Ultrafast Optical Sources, Electron Microscopy, Materials Synthesis, Proximal Probes, Theory and Computing, and CFN Endstations at NSLS. The CFN

[a] The full project TEC and TPC, established at Critical Decision 2 (Approve Performance Baseline), are $79,700,000 and $81,000,000 respectively, and include the cost for PED from project 02-SC-002.

will allow users to control processes, tailoring the properties of materials structured on the nanoscale. Some of these materials, all relevant to the BES mission, include piezoelectrics, ferroelectrics, organic films and conductors, magnetic nanocomposites, and catalysts.

The preliminary engineering and detailed engineering design necessary to construct a BNL Center for Functional Nanomaterials have been completed. The engineering effort included all engineering phase activities, including field investigation, preliminary design, specifications and drawings for conventional construction, final design, preparation of procurement documents for experimental equipment, and construction/equipment procurement estimates.

The completed design will enable construction of a new two-story Laboratory/Office building of approximately 94,500 gross square feet. The facility will include clean rooms, general laboratories, wet and dry laboratories for sample preparation, fabrication, and analysis. Included will be some of the equipment necessary to explore, manipulate and fabricate nanoscale materials and structures. Also included are individual offices and landscape office areas, seminar area, transient user space for visiting collaborators with access to computer terminals, conference areas on both floors, and vending/lounge areas. In addition, it will include circulation/ancillary space, including mechanical equipment areas, corridors, and other support spaces.

Technical procurement for the project will include an initial suite of laboratory equipment for the CFN laboratory themes: Nanopatterning, Ultrafast Optical Sources, Electron Microscopy, Materials Synthesis, Proximal Probes, and Theory and Computing as well as for the designated CFN Endstations at NSLS.

The building will incorporate human factors into its design to encourage peer interactions and collaborative interchange by BNL staff and CFN users and visitors. In addition to flexible office and laboratory space it will provide "interaction areas," a seminar room and a lunch room for informal discussions. This design approach is considered state-of-the-art in research facility design as it leverages opportunities for the free and open exchange of ideas essential to creative research processes.

The FY 2005 funds were used to begin conventional construction and technical equipment procurement. FY 2006 funds are being used to continue conventional construction and technical equipment procurement. The FY 2007 funds will be used to complete the building construction and procure additional technical equipment.

The project will be conducted in accordance with the project management requirements in DOE Order 413.3 and DOE Manual 413.3-1, Program and Project Management for the Acquisition of Capital Assets.

### Compliance with Project Management Order

- Critical Decision-0: Approve Mission Need—3Q FY 2002
- Critical Decision-1: Approve Preliminary Baseline Range—4Q FY 2003
- External Independent Review (EIR) Final Report—April 28, 2004
- Critical Decision-2: Approve Performance Baseline—3Q FY 2004
- Critical Decision-3: Approve Start of Construction—4Q FY 2005
- Critical Decision-4a: Approve Building Occupation—3Q FY 2007
- Critical Decision-4b: Approve Start of Operations—3Q FY 2008

## 5. Financial Schedule (dollars in thousands)

| | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design/Construction by Fiscal Year | | | |
| Design | | | |
| 2003 | 988[a] | 988[a] | 733 |
| 2004 | 2,982[a] | 2,982[a] | 2,721 |
| 2005 | 1,996[a] | 1,996[a] | 1,555 |
| 2006 | — | — | 957 |
| Total, Design PED (02-SC-002) | 5,966 | 5,966 | 5,966 |
| Construction | | | |
| 2005 | 18,317[b] | 18,317[b] | 772 |
| 2006 | 36,187[b] | 36,187[b] | 34,079 |
| 2007 | 18,864[b] | 18,864[b] | 36,738 |
| 2008 | 366[b] | 366[b] | 2,145 |
| Total, Construction | 73,734 | 73,734 | 73,734 |
| Total, TEC | 79,700 | 79,700 | 79,700 |

## 6. Details of Project Cost Estimate

## Total Estimated Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Preliminary and Final Design (PED 02-SC-002) | 5,966 | 5,966 |
| Construction Phase | | |
| Site Preparation | 1,920 | 5,392 |
| Equipment | 21,279 | 26,097 |
| All other construction | 39,922 | 31,379 |
| Contingency | 10,613 | 10,866 |
| Total, Construction | 73,734 | 73,734 |
| Total, TEC | 79,700 | 79,700 |

[a] PED funding was reduced $12,000 as a result of the FY 2003 general reduction and rescission and by $18,000 as a result of the FY 2004 rescission. This total reduction/rescission is restored in FY 2005 and FY 2006 to maintain the TEC and project scope. A rescission reduced FY 2005 PED funding by $16,000.

[b] Construction funding was reduced by $148,000 as a result of the FY 2005 rescission and by $366,000 as a result of the FY 2006 rescission. This total reduction is restored in FY 2007 and FY 2008 to maintain the TEC and project scope.

## Other Project Costs

| | (dollars in thousands) | |
|---|---|---|
| | Current Estimate | Previous Estimate |
| Conceptual Planning | 300 | 300 |
| Start-up | 1,000 | 1,000 |
| Total, OPC | 1,300 | 1,300 |

## 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC(Design) | 5,966 | — | — | — | — | — | — | 5,966 |
| TEC (Construction) | 34,851 | 36,738 | 2,145 | — | — | — | — | 73,734 |
| OPC Other than D&D | 300 | 475 | 525 | — | — | — | — | 1,300 |
| Total, Project Costs | 41,117 | 37,213 | 2,670 | — | — | — | — | 81,000 |

## 8. Related Operations and Maintenance Funding Requirements

| | |
|---|---|
| Start of Operation or Beneficial Occupancy (fiscal quarter) | 3Q FY 2008[a] |
| Expected Useful Life (number of years) | 40 |
| Expected Future start of D&D for new construction (fiscal quarter) | N/A |

## (Related Funding Requirements)

(dollars in thousands)

| | Annual Costs | | Life cycle costs | |
|---|---|---|---|---|
| | Current estimate | Prior Estimate | Current estimate | Prior Estimate |
| Operations | 17,500 | — | — | — |
| Maintenance | 1,000 | — | — | — |
| Total Related funding | 18,500 | — | 821,000 | — |

## 9. Required D&D Information

Not applicable.

## 10. Acquisition Approach

Design and inspection of the facilities and equipment will be by the operating contractor and A/E subcontractor as appropriate. Technical construction will be competitively bid, lump sum contracts. To the extent feasible, construction and procurement will be accomplished by fixed-price contracts awarded on the basis of competitive bidding.

[a] Experimental research will begin at the time of Beneficial Occupancy of the facility. These research costs are not part of the TPC and will be provided by BES.

# 04-R-313, Molecular Foundry
# Lawrence Berkeley National Laboratory, Berkeley, California

## 1. Significant Changes

There have been no significant changes to scope, cost, or schedule.

## 2. Design, Construction and D&D Schedule

(fiscal quarter)

| | Preliminary Design Start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2006 ............ | 3Q 2002 | 1Q 2004 | 2Q 2004 | 1Q 2007 | N/A | N/A |
| FY 2007 ............ | 3Q 2002 | 1Q 2004 | 2Q 2004 | 1Q 2007 | N/A | N/A |

## 3. Baseline and Validation Status

(dollars in thousands)

| | TEC | OPC, except D&D Costs | Offsetting D&D Costs | Total Project Costs | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2006 ............. | 83,700 | 1,300 | — | 85,000 | 85,000 | N/A |
| FY 2007 ............. | 83,604[a] | 1,300 | — | 84,904[a] | 84,904 | N/A |

## 4. Project Description, Justification and Scope

The Molecular Foundry at LBNL will be a new structure near the National Center for Electron Microscopy. The project includes an approximately 89,000 gross square foot research building, a separate approximately 6,000 gross square foot utility center, and an initial set of special equipment to support nanoscale scientific research. The research building will be an advanced facility with state-of-the-art clean rooms for the design, modeling, synthesis, processing, fabrication and characterization of novel molecules and nanoscale materials. Space in the new facility will support studies in nanostructures by providing offices and laboratories for materials science, physics, chemistry, biology, and molecular biology. These laboratories, equipped with advanced instrumentation and staffed by full-time, dedicated staff scientists and technicians, will be user facilities, available to scientists from universities, industry, and government laboratories whose research proposals will have been peer reviewed by a Proposal Study Panel. This combination of advanced equipment, collaborative staff, and breadth across disciplines will allow users to explore the frontiers of nanoscience.

The goals and operation of the Molecular Foundry are consistent with DOE guidance and address the research challenges described in the reports *Nanoscale Science, Engineering and Technology Research Directions and Complex Systems: Science for the 21st Century*. The Foundry's laboratories will be designed and constructed to facilitate collocation of research activities in a wide variety of fields, as required for progress in this new area of science. The Foundry will support a broad research effort

[a] The TEC and TPC have been reduced by $96,000 due to the FY 2006 rescission, and includes the costs for PED from project 02-SC-002.

focusing on both "hard" nanomaterials (nanocrystals, tubes, and lithographically patterned structures) and "soft" nanometer-sized materials (polymers, dendrimers, DNA, proteins, and whole cells), as well as design, fabrication, and study of multi-component, complex, functional assemblies of such materials.

By functioning as a "portal" to Lawrence Berkeley National Laboratory's established major user facilities, the Foundry will also leverage existing nanoscience research capabilities at the Advanced Light Source, the National Center for Electron Microscopy, and the National Energy Research Scientific Computing Center. The research program will, as an additional benefit, provide significant educational and training opportunities for students and postdoctoral fellows as the "first true generation" of nanoscientists.

FY 2004 funding was used to initiate construction to complete site preparation, and for equipment procurement. FY 2005 and FY 2006 funding is being used to complete conventional construction and begin equipment procurement. FY 2007 funding will be used to complete equipment procurement and installation.

## 5. Financial Schedule

(dollars in thousands)

| | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design/Construction by Fiscal Year | | | |
| Design | | | |
| 2002 | 500 | 500 | 38 |
| 2003 | 6,715[a] | 6,715[a] | 5,263 |
| 2004 | — | — | 1,896 |
| 2005 | — | — | 18 |
| Total, Design (PED No. 02-SC-002) | 7,215 | 7,215 | 7,215 |
| Construction | | | |
| 2004 | 34,794[b] | 34,794[b] | 10,970 |
| 2005 | 31,828[bc] | 31,828[bc] | 37,626 |
| 2006 | 9,510[cd] | 9,510[cd] | 26,923 |
| 2007 | 257[c] | 257[c] | 870 |
| Total, Construction | 76,389 | 76,389 | 76,389 |
| Total TEC | 83,604 | 83,604 | 83,604 |

[a] PED funding was reduced by $85,000 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission was restored in FY 2005 to construction to maintain the TEC and project scope.
[b] Construction funding was reduced by $207,000 as a result of the FY 2004 rescission and by $257,000 as a result of the FY 2005 rescission.
[c] This total reduction is restored FY 2006 and FY 2007 to maintain the TEC and project scope.
[d] Construction was reduced by $96,000 as a result of the FY 2006 rescission.

# 6. Details of Project Cost Estimate

## Total Estimated Costs

| | (dollars in thousands) | |
|---|---|---|
| | Current Estimate | Previous Estimate |
| Preliminary and Final Design (PED 02-SC-002) | 7,215 | 7,215 |
| Construction Phase | | |
| Building & Improvements to land | 52,106 | 49,444 |
| Special Equipment[a] | 17,082 | 15,056 |
| All other construction | 4,236 | 3,863 |
| Contingency | 2,965 | 8,122 |
| Total, Construction | 76,389 | 76,485 |
| Total, TEC | 83,604 | 83,700 |

## Other Project Costs

| | (dollars in thousands) | |
|---|---|---|
| | Current Estimate | Previous Estimate |
| Conceptual Planning | 932 | 932 |
| Start-up | 368 | 368 |
| Total, OPC | 1,300 | 1,300 |

# 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC (Design) | 7,215 | — | — | — | — | — | — | 7,215 |
| TEC (Construction) | 75,519 | 870 | — | — | — | — | — | 76,389 |
| OPC Other than D&D | 1,300 | — | — | — | — | — | — | 1,300 |
| Total Project Costs | 84,034 | 870 | — | — | — | — | — | 84,904 |

[a] Initial research equipment.

## 8. Related Operations and Maintenance Funding Requirements

| | |
|---|---|
| Start of Operation or Beneficial Occupancy (fiscal year)................................... | 1Q FY 2007[a] |
| Expected Useful Life (number of years)............................................................. | 40 |
| Expected Future start of D&D for new construction (fiscal year)....................... | N/A |

## (Related Funding Requirements)

(dollars in thousands)

| | Annual costs | | Life cycle costs | |
|---|---|---|---|---|
| | Current Estimate | Previous Estimate | Current Estimate | Previous Estimate |
| Operations .................................... | 18,105 | N/A | — | N/A |
| Maintenance ................................. | 395 | N/A | — | N/A |
| Total Related funding.................... | 18,500 | N/A | 835,000 | N/A |

## 9. Required D&D Information

Not applicable. This project received construction funding starting in FY 2004. The project includes 95,000 gsf of new construction which was offset by banked excess space that had been previously eliminated.

## 10. Acquisition Approach

An Architect Engineering firm (AE) with appropriate multi-disciplinary design experience has prepared a building program and design criteria with the support of the LBNL Facilities Department. The AE also prepared preliminary and final design and is providing technical oversight during construction. A Construction Management (CM) contractor performed cost, schedule, and constructability reviews during design. Selection of the CM contractor during the design phases was based on competitive bidding of the Construction General Conditions. The CM contract had an option for management of the construction process. At the completion of design, the CM contractor bid out the design to subcontractors. The University has exercised its option to proceed with the CM contractor. Construction subcontract(s) were awarded on a competitive basis using best value source selection criteria that included price, safety, and other considerations.

[a] Fiscal quarter designated corresponds to start of full operations and completion of project. Initial operations (experimental research) with a limited suite of special equipment will begin earlier; these research costs are not part of the TPC and will be funded by the BES program.

# 03-SC-002, Project Engineering and Design (PED), Linac Coherent Light Source, Stanford Linear Accelerator Center

## 1. Significant Changes

There have been no significant changes to scope, cost, or schedule.

## 2. Design, Construction, and D&D Schedule

(fiscal quarter)

| | Preliminary Design Start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2006 ..... | 2Q FY 2003 | 4Q FY 2006 | N/A | N/A | N/A | N/A |
| FY 2007 ..... | 2Q FY 2003 | 4Q FY 2006 | N/A | N/A | N/A | N/A |

## 3. Baseline and Validation Status[a]

(dollars in thousands)

| | TEC | OPC, except D&D Costs | Offsetting D&D Costs | Total Project Costs | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2006 ..... | 36,000 | 7,500 | — | 43,500 | N/A | N/A |
| FY 2007 ..... | 35,974[b] | 7,500 | — | 43,474[b] | N/A | N/A |

## 4. Project Description, Justification and Scope

These funds allowed the Linac Coherent Light Source (LCLS), located at the Stanford Linear Accelerator Center (SLAC), to proceed from conceptual design into preliminary design and definitive design. The design effort has been sufficient to assure project feasibility, define the scope, provide detailed estimates of construction costs based on the approved design, working drawings and specifications, and provide construction schedules including procurements. The design effort has ensured that long-lead procurement items could be initiated and construction could physically start to support the baseline LCLS schedule.

The purpose of the LCLS Project is to provide laser-like radiation in the x-ray region of the spectrum that is 10 billion times greater in peak brightness than any existing coherent x-ray light source. This advance in brightness is similar to that of a synchrotron over a 1960's laboratory x-ray tube. Synchrotrons revolutionized science across disciplines ranging from atomic physics to structural biology. Advances from the LCLS are expected to be equally dramatic. The LCLS Project will provide the first demonstration of an x-ray free-electron-laser (FEL) in the 1.5–15 Angstrom range and will apply these extraordinary, high-brightness x-rays to an initial set of scientific problems. This will be the world's first such facility.

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[a] Construction funding for this project is included in project 05-R-320. The estimates in section 3 are for PED only. The full project TEC and TPC, established at Critical Design 2 (Approve Performance Baseline), are $315,000,000 and $379,000,000, respectively.

[b] The TEC and TPC have been reduced by $26,000 due to the FY 2006 rescission.

The LCLS is based on the existing SLAC linac. The SLAC linac can accelerate electrons or positrons to 50 GeV for colliding beam experiments and for nuclear and high-energy physics experiments on fixed targets. At present, the first two-thirds of the linac is being used to inject electrons and positrons into PEP-II, and the entire linac is used for fixed target experiments. When the LCLS is completed, the latter activity will be limited to 25 percent of the available beam time and the last one-third of the linac will be available for the LCLS a minimum of 75 percent of the available beam time. For the LCLS, the linac will produce high-brightness 5–15 GeV electron bunches at a 120 Hz repetition rate. When traveling through the new 120-meter long LCLS undulator, these electron bunches will amplify the emitted x-ray radiation to produce an intense, coherent x-ray beam for scientific research.

The LCLS makes use of technologies developed for the SLAC and the next generation of linear colliders, as well as the progress in the production of intense electron beams with radiofrequency photocathode guns. These advances in the creation, compression, transport, and monitoring of bright electron beams make it possible to base this next generation of x-ray synchrotron radiation sources on linear accelerators rather than on storage rings.

The LCLS will have properties vastly exceeding those of current x-ray sources (both synchrotron radiation light sources and so-called "table-top" x-ray lasers) in three key areas: peak brightness, coherence (i.e., laser-like properties), and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing over $10^{11}$ x-ray photons in a pulse with duration of less than 230 femtoseconds. These characteristics of the LCLS will open new realms of scientific applications in the chemical, material, and biological sciences. The LCLS Scientific Advisory Committee, working in coordination with the broad scientific community, identified high priority initial experiments that are summarized in the document, *LCLS: The First Experiments*. These first five areas of experimentation are: fundamental studies of the interaction of intense x-ray pulses with simple atomic systems; use of the LCLS to create warm dense matter and plasmas; structural studies on single nanoscale particles and biomolecules; ultrafast dynamics in chemistry and solid-state physics; and studies of nanoscale structure and dynamics in condensed matter.

The experiments fall into two classes. The first follows the traditional role of x-rays to probe matter without modifying it, while the second utilizes the phenomenal intensity of the LCLS to excite matter in fundamentally new ways and to create new states in extreme conditions. The fundamental studies of the interactions of intense x-rays with simple atomic systems are necessary to lay the foundation for all interactions of the LCLS pulse with atoms embedded in molecules and condensed matter. The structural studies of individual particles or molecules make use of recent advances in imaging techniques for reconstructing molecular structures from diffraction patterns of non-crystalline samples. The enormous photon flux of the LCLS may make it feasible to determine the structure of a *single* biomolecule or small nanocrystal using only the diffraction pattern from a single moiety. This application has enormous potential in structural biology, particularly for important systems such as membrane proteins, which are virtually uncharacterized by x-ray crystallography because they are nearly impossible to crystallize. The last two sets of experiments make use of the extremely short pulse of the LCLS to follow dynamical processes in chemistry and condensed matter physics in real time. The use of ultrafast x-rays will open up entire new regimes of spatial and temporal resolution to both techniques.

The LCLS Project requires a 135 MeV injector to be built at Sector 20 of the 30-sector SLAC linac to create the electron beam required for the x-ray FEL. The last one-third of the linac will be modified by adding two magnetic bunch compressors. Most of the linac and its infrastructure will remain unchanged. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new undulator and associated equipment. Two new buildings, the Near Experimental Hall and the Far Experimental Hall will be constructed and connected by a beam line tunnel. A Central Laboratory and Office Building will be constructed to provide laboratory and office space for LCLS users and serve as a center of excellence for basic research in x-ray physics and ultrafast science.

The project is being conducted in accordance with the project management requirements in DOE Order 413.3 -1, Program and Project Management for the Acquisition of Capital Assets.

**Compliance with Project Management Order**

- Critical Decision-0: Approve Mission Need—3Q FY 2001
- Critical Decision-1: Approve Preliminary Baseline Range—1Q FY 2003
- Critical Decision-2a: Approve Long-Lead Procurement Budget—3Q FY 2003
- Critical Decision-2b: Approve Performance Baseline—3Q FY 2005
- External Independent Review Final Report—3Q FY 2005
- Critical Decision 3a: Approve Start of Long-Lead Procurement—1Q FY 2005
- Critical Decision-3b: Approve Start of Construction—2Q FY 2006
- Critical Decision-4: Approve Start of Operations—2Q FY 2009

## 5. Financial Schedule (dollars in thousands)

| | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design by Fiscal Year | | | |
| 2003 | 5,925 [a] | 5,925 [a] | 3,644 |
| 2004 | 7,456 [a] | 7,456 [a] | 9,713 |
| 2005 | 19,914 [a] | 19,914 [a] | 18,388 |
| 2006 | 2,518 [ab] | 2,518 [ab] | 4,056 |
| 2007 | 161 [a] | 161 [a] | 173 |
| Total, Design PED (03-SC-002) | 35,974 | 35,974 | 35,974 |

[a] PED funding was reduced as a result of the FY 2003 general reduction and rescission by $75,000, as a result of the FY 2004 rescission by $44,000, and as a result of the FY 2005 rescission by $161,000. This total reduction is restored in FY 2005, FY 2006, and FY 2007 to maintain the TEC and project scope.

[b] PED funding was reduced by $26,000 as a result of the FY 2006 rescission.

## 6. Details of Project Cost Estimate

## Total Estimated Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Preliminary and Final Design | 35,974 | 35,974 |

## Other Project Costs

(dollars in thousands)

| | Current Estimate | Previous Estimate |
|---|---|---|
| Conceptual Planning | 1,500 | 1,500 |
| R&D | 6,000 | 6,000 |
| Total, OPC | 7,500 | 7,500 |

## 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC (Design) | 35,801 | 173 | — | — | — | — | — | 35,974 |
| OPC (Design) | 7,500 | — | — | — | — | — | — | 7,500 |
| Total, Project Costs | 43,301 | 173 | — | — | — | — | — | 43,474 |

## 8. Related Operations and Maintenance Funding Requirements

Not applicable for project engineering and design.

## (Related Funding Requirements)

Not applicable for project engineering and design.

## 9. Required D&D Information

Not applicable for project engineering and design.

## 10. Acquisition Approach

A Conceptual Design Report (CDR) for the project was completed and reviewed in FY 2002. Key design activities are being specified in the areas of the injector, undulator, x-ray optics and experimental halls to reduce schedule risk to the project and expedite the startup. Also, the LCLS management systems have been being put in place and tested during the Project Engineering and Design (PED) phase. These activities are managed by the LCLS Project Office at SLAC, with additional portions of the project being executed by staff at Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL).

The design of technical systems is being accomplished by the three collaborating laboratories. The conventional construction design aspect (experimental halls, tunnel connecting the halls, and a Central Laboratory and Office Building) was contracted to an experienced Architect/Engineering (A/E) firm to perform preliminary and final design. Preliminary design was completed in FY 2004. Final design began in FY 2005 and will be complete by the end of FY 2006.

# 03-R-313[a], The Center for Integrated Nanotechnologies (CINT) Facility Sandia National Laboratories, Albuquerque, New Mexico, and Los Alamos National Laboratory, Los Alamos, New Mexico

## 1. Significant Changes

There have been no significant changes to scope, cost, or schedule.

## 2. Design, Construction, and D&D Schedule

(fiscal quarter)

| | Preliminary Design start | Final Design Complete | Physical Construction Start | Physical Construction Complete | D&D Offsetting Facilities Start | D&D Offsetting Facilities Complete |
|---|---|---|---|---|---|---|
| FY 2006… | 4Q FY 2002 | 2Q FY 2004 | 1Q FY 2004 | 3QFY 2007 | N/A | N/A |
| FY 2007… | 4Q FY 2002 | 2Q FY 2004 | 1Q FY 2004 | 3Q FY 2007 | N/A | N/A |

## 3. Baseline and Validation Status

(dollars in thousands)

| | TEC | OPC, except D&D Costs | Offsetting D&D Costs | Total Project Costs | Validated Performance Baseline | Preliminary Estimate |
|---|---|---|---|---|---|---|
| FY 2006... | 73,800 | 2,000 | — | 75,800 | 75,800 | N/A |
| FY 2007... | 73,754[b] | 2,000 | — | 75,754[b] | 75,754 | N/A |

## 4. Project Description, Justification, and Scope

This project provides materials and services required to design and construct the proposed Center for Integrated Nanotechnologies (CINT) Facility. CINT is one of the five BES/Office of Science Nanoscale Science Research Centers (NSRCs). It will be operated jointly by Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL). CINT is a U.S. Department of Energy (DOE) line item project that is being carried out as a partnership between SNL and LANL to design and build a world-class user facility for research in nanoscale science. The partnership between two world-class DOE laboratories, each with significant technical expertise and capability in nanoscale research, will provide the best possible facility to the nanoscience research community.

CINT will be a distributed Center that is jointly operated by SNL and LANL. Its primary objective is to develop the scientific principles that govern the performance and integration of nanoscale materials, thereby building the foundations for future nanotechnologies. The distinguishing characteristic of the Center is its focus on exploring the path from scientific discovery to the integration of nanostructures into the micro and macro worlds. This path involves experimental and theoretical exploration of behavior, understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures. This Center works closely with the other NSRCs to ensure that their

[a] This project was submitted in the FY 2004 President's Request as project 04-R-314. In FY 2003 Congress appropriated construction funds for this project (after the FY 2004 Request was submitted to Congress) under project 03-R-313.
[b] The full project TEC and TPC established at Critical Decision 2 (Approve Performance Baseline) are $73,754,000 and $75,754,000, respectively and include the costs for PED from project 02-SC-002. TEC and TPC are reduced by $46,000 as a result of the FY 2006 rescission.

discoveries are evaluated in the context of integrated functional systems. This approach offers a unique role for the DOE in support of the National Nanotechnology Initiative.

The managements of the Los Alamos and Sandia National Laboratories are committed to develop CINT as a DOE national resource for the advancement of nanoscience and technology. Through its laboratory partnership, CINT will leverage expertise and facilities from both SNL and LANL and make those resources available to the user community. In order to provide a strong central focus for the user community while also providing extraordinary leverage and access to existing laboratory capabilities, the CINT project, in conjunction with its user community, has developed a unique Core/Gateway structure.

The Core Facility (approximately 95,000 gross square feet), which will be constructed in Albuquerque, will be the single point of entry for the CINT user community and will provide the multi-disciplinary research environment needed to explore scientific challenges associated with nanoscience integration. In order to assure open access to the user community, the Core Facility is being constructed on DOE property outside of the Kirtland Air Force Base (KAFB).

In addition to developing the Core Facility, the CINT user community strongly recommended that the CINT project also provide access to the deep and broad resources of both SNL and LANL. The Gateway Facilities at both SNL and LANL are designed to provide the user community with direct access to existing DOE/SC and DOE/NNSA programmatic investments at each laboratory.

The Gateway to Sandia Facility is housed within an existing space in an NNSA building located on the main campus within the KAFB. The Gateway to Sandia, which will provide office and laboratory space for CINT users, is co-located with many of Sandia’s existing facilities for nanoscale science research and Sandia’s world-class microfabrication facilities. No new construction is required for the Gateway to Sandia since it will utilize existing NNSA space. (While the NNSA facility that houses the Gateway to Sandia is within the KAFB boundaries, it is located outside classified restricted boundaries and is therefore open for general user access).

Development of the Gateway to Los Alamos Facility (approximately 34,000 gross square feet) involves the construction of a new building on the Los Alamos campus providing the user community direct access to existing nanoscale materials science and bioscience capabilities. The Gateway to Los Alamos Facility is located in the center of the Los Alamos materials science complex which is in an open security environment and will facilitate easy access to these existing nanoscale materials science and bioscience resources. Traditionally, materials science and bioscience have been viewed as separate activities and are housed primarily in separate parts of the Los Alamos campus. The Gateway to Los Alamos will provide a unique research environment for CINT users by combining nanoscale materials science and biosciences capabilities and expertise under one roof surrounded by supporting resources accessible to CINT users.

The CINT project is building a unified community around its Core Facility and two Gateway Facilities (one each at SNL and LANL). The CINT project is using public workshops, presentations at scientific forums, web-based communications, and one-on-one interactions with CINT scientists to help build its user community with significant participation from university, industrial, and laboratory researchers. Input and advice from the user community is used to help define and refine the proper tools and scientific focus to address the challenges of nanoscale science and technology. CINT is focused on *integration* because it is the key factor in the scientific development and application of nanoscience. The tools and resources of CINT will be available at no cost to university, industrial, and laboratory researchers through a peer-reviewed process. The external scientific community has been and will continue to be a vital partner in developing CINT so that it is successful in achieving its vision.

The initial technical focus of the Center will be on the following five thrusts:

- Nanophotonics and Nanoelectronics
- Complex Functional Nanomaterials
- Nanomechanics
- Nanoscale and Bio-Microinterfaces
- Theory and Simulation

This laboratory and office space complex will house state-of-the-art clean rooms and equipment for nanolithography, atomic layer deposition, and materials characterization along with general purpose chemistry and electronics labs and offices for Center staff and collaborators.

The CINT Core Facility will include class 1,000 clean room space for nanofabrication and characterization equipment and class 100 clean room space for lithography activities. This facility will also require general purpose chemistry/biology laboratories, electronic and physical measurement laboratories, office and meeting room space.

The scope of this project is to construct the CINT Core and Gateway to Los Alamos. The engineering effort includes preliminary and final design of both buildings. The project also includes procurement of an initial set of experimental capital equipment and construction of facilities. FY 2003, FY 2004, and FY 2005 construction funds were used for conventional construction and equipment procurement. FY 2006 and FY 2007 construction funds will be used to continue these activities.

The project will be conducted in accordance with the project management requirements in DOE Order 413.3 and DOE Manual 413.3-1, Program and Project Management for the Acquisition of Capital Assets.

**Compliance with Project Management Order**

- Critical Decision-0: Approve Mission Need—3Q FY 2001
- Critical Decision-1: Approve Preliminary Baseline Range—3Q FY 2002
- Critical Decision-2: Approve Performance Baseline—4Q FY 2003
- External Independent Review Final Report—4Q FY 2003
- Critical Decision-3: Approve Start of Construction—1Q FY 2004
- Critical Decision-4a: Approve Start of Initial Operations—3Q FY 2006
- Critical Decision-4b: Approve Start of Full Operations—3Q FY 2007

## 5. Financial Schedule

| (dollars in thousands) | Appropriations | Obligations | Costs |
|---|---|---|---|
| Design/Construction by Fiscal Year | | | |
| Design | | | |
| 2002 | 1,000 | 1,000 | 167 |
| 2003 | 3,159[a] | 3,159[a] | 3,319 |
| 2004 | — | — | 562 |
| 2005 | — | — | 111 |
| Total, Design PED (02-SC-002) | 4,159 | 4,159 | 4,159 |
| Construction | | | |
| 2003 | 4,444[b] | 4,444[b] | — |
| 2004 | 29,674[b] | 29,674[b] | 6,946 |
| 2005 | 30,650[ab] | 30,650[ab] | 40,857 |
| 2006 | 4,580[bc] | 4,580[bc] | 15,330 |
| 2007 | 247[b] | 247[b] | 6,462 |
| Total, Construction | 69,595 | 69,595 | 69,595 |
| Total TEC | 73,754 | 73,754 | 73,754 |

## 6. Details of Project Cost Estimate

## Total Estimated Costs

| (dollars in thousands) | Current Estimate | Previous Estimate |
|---|---|---|
| Preliminary and Final Design(PED 02-SC-002) | 4,159 | 4,159 |
| Construction Phase | | |
| Site Preparation | 1,430 | 1,430 |
| Equipment | 14,002 | 13,861 |
| All other construction | 48,950 | 45,158 |
| Contingency | 5,213 | 9,192 |
| Total, Construction Costs | 69,595 | 69,641 |
| Total, TEC | 73,754 | 73,800 |

[a] PED funding was reduced $41,000 as a result of the FY 2003 general reduction and rescission. This total reduction/rescission was restored to construction in FY 2005 to maintain the TEC and project scope.

[b] Construction funding was reduced by $56,000 as a result of the FY 2003 general reduction and rescission, by $176,000 as a result of the FY 2004 rescission, and by $247,000 as a result of the FY 2005 rescission. This total reduction is restored in FY 2005, FY 2006, and FY 2007 to maintain the TEC and project scope.

[c] Construction funding was reduced by $46,000 as a result of the FY 2006 rescission.

## Other Project Costs

| | (dollars in thousands) | |
|---|---|---|
| | Current Estimate | Previous Estimate |
| Conceptual Planning | 800 | 800 |
| Start-up | 1,200 | 1,200 |
| Total, OPC | 2,000 | 2,000 |

## 7. Schedule of Project Costs

(dollars in thousands)

| | Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | Outyears | Total |
|---|---|---|---|---|---|---|---|---|
| TEC (Design) | 4,159 | — | — | — | — | — | — | 4,159 |
| TEC (Construction) | 63,133 | 6,462 | — | — | — | — | — | 69,595 |
| OPC Other than D&D | 2,000 | — | — | — | — | — | — | 2,000 |
| Total Project Costs | 69,292 | 6,462 | — | — | — | — | — | 75,754 |

## 8. Related Operations and Maintenance Funding Requirements

| | |
|---|---|
| Start of Operation or Beneficial Occupancy (fiscal quarter) | 3Q FY 2007[a] |
| Expected Useful Life (number of years) | 40 |
| Expected Future start of D&D for new construction (fiscal quarter) | N/A |

## (Related Funding Requirements)

(dollars in thousands)

| | Annual Costs | | Life Cycle Costs | |
|---|---|---|---|---|
| | Current estimate | Previous Estimate | Current estimate | Previous Estimate |
| Operations | 18,000 | N/A | — | N/A |
| Maintenance | 500 | N/A | — | N/A |
| Total Related funding | 18,500 | N/A | 830,800 | N/A |

## 9. Required D&D Information

Not applicable. This project received construction funding starting in FY 2003. The project includes approximately 95,000 gsf of new construction at SNL and approximately 34,000 gsf of new construction at LANL, which was offset by banked excess space.

[a] Fiscal quarter designated corresponds to start of full operations and completion of project. Initial operations (experimental research) with a limited suite of special equipment will begin earlier; these research costs are not part of the TPC and will be funded by the BES program.

## 10. Acquisition Approach

Preliminary and final design for the Core Facility was accomplished through the use of a firm fixed-price contract with a qualified and experienced A/E firm. The selection was made under the SNL Best Value Contracting Procedures. The construction contract for the Core Facility has been awarded under a fixed-price contract using the SNL Best Value Contracting Procedures.

The design and construction of the Gateway to Los Alamos Facility is being accomplished through the use of a firm fixed-price Design-Build contract with a qualified and experienced construction-A/E firm. The selection was made under the LANL Best Value Contracting Procedures using LANL developed Performance Specifications to solicit proposals from interested firms.

Procurement of the initial set of experimental capital equipment for both facilities is being carried out at SNL using standard corporate procurement processes. Fixed price contracts are awarded for the instruments after Best Value Contracting Procedures are used to select the vendors.

# Advanced Scientific Computing Research

## Funding Profile by Subprogram

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

**Public Law Authorizations:**
Public Law 95-91, "Department of Energy Organization Act"
Public Law 103-62, "Government Performance and Results Act of 1993"
Public Law 108-423, "Department of Energy High-End Computing Revitalization Act of 2004"
Public Law 109-58, "Energy Policy Act of 2005"

### Mission

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

### Benefits

ASCR supports DOE's mission to provide world-class scientific research capacity through peer-reviewed scientific results in mathematics, high performance computing and advanced networks, and through the application of computers capable of many trillions of operations per second (terascale computers) to advanced scientific applications. Computer-based simulation enables us to understand and predict the behavior of complex systems that are beyond the reach of our most powerful experimental probes or our most sophisticated theories. Computational modeling has greatly advanced our understanding of fundamental processes of nature, such as fluid flow and turbulence or molecular structure and reactivity. Through modeling and simulation, we will be able to explore the interior of stars to understand how the chemical elements were created and learn how protein machines work inside living cells, which could enable us to design microbes that address critical waste cleanup problems. We can design novel catalysts and high-efficiency engines that could expand our economy, lower pollution, and reduce our dependence on foreign oil. Computational science is increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering.

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

## Strategic and Program Goals

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

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

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

Program Goal 05.23.00.00: Deliver forefront computational and networking capabilities—Deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.

### Contribution to Program Goal 05.23.00.00 (Deliver forefront computational and networking capabilities)

The ASCR program contributes to Program Goal 05.23.00.00 by delivering the fundamental mathematical and computer science research that enables the simulation and prediction of complex physical and biological systems, providing the advanced computing capabilities needed by researchers to take advantage of this understanding, and delivering the fundamental networking research and facilities that link scientists across the nation to the computing and experimental facilities and their colleagues to enable scientific discovery. ASCR supports fundamental research in applied mathematics, computer science, computer networks, and tools for electronic collaboration; integrates the results of these basic research efforts into tools and software that can be used by scientists in other disciplines, especially through efforts such as Scientific Discovery through Advanced Computing (SciDAC); and provides the advanced computing and network resources that enable scientists to use these tools to deliver extraordinary science. Applied Mathematics enables scientists to build models of physical and natural systems with extraordinary fidelity, and provides the algorithms the computer requires to manipulate that representation of the world effectively, exposing the underlying structure. Computer science research provides the link between the mathematics and the actual computer systems. Finally, scientific discovery results from simulations conducted on the advanced computers themselves, including experimental computers with hardware designs optimized to enable particular types of scientific applications, and the largest computing capabilities available to the general scientific community. All of these elements are critical to advance the frontiers of simulation. Shrinking the distance between scientists and the resources they need is also critical to SC. The challenges that SC faces require teams of scientists distributed across the country, as well as the full national portfolio of experimental and computational tools. High performance networks and network research provide the capability to move the millions of gigabytes that these resources generate to the scientists' desktops.

Therefore, the ASCR program contributes to General Goal 5 by enabling research programs across SC, as well as other elements of the Department, to succeed. The following indicators establish specific long term (10 years) goals in Scientific Advancement that the ASCR program is committed to, and progress can be measured against:

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

## Funding by General and Program Goal

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

## Annual Performance Results and Targets

| FY 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Program Goal 05.23.00.00 Deliver forefront computational and networking capabilities | | | | | |
| Mathematical, Information and Computational Sciences | | | | | |
| | Began installation of next generation National Energy Research Scientific Computing Center (NERSC) computer, NERSC-4, that will at least double the capability available in FY 2002 to solve leading edge scientific problems. [Goal Not Met] | Maintained Procurement Baselines. Percentages within (1) original baseline cost for completed procurements of major computer systems or network services, and (2) original performance baseline versus integrated performance over the life of the contracts. [Goal Met] | Maintained Procurement Baselines. Percentages within (1) original baseline cost for completed procurements of major computer systems or network services, and (2) original performance baseline versus integrated performance over the life of the contracts. [Goal Met] | | |
| | Initiated at least 5 competitively selected interdisciplinary research teams to provide computational science and applied mathematics advances that will accelerate biological discovery in microbial systems and develop the next generation of computational tools required for nanoscale science based on peer review, in partnership with the Biological and Environmental Research (BER) and Basic Energy Sciences (BES) programs, respectively, of submitted proposals. [Goal Met] | Improved Computational Science Capabilities. Average annual percentage increased in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. [Goal Met] | Improved Computational Science Capabilities. Average annual percentage increased in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. [Goal Met] | Improve Computational Science Capabilities. Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. FY 2006— >50% | Improve Computational Science Capabilities. Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. FY 2007— >50% |
| | Maintained and operated facilities, including NERSC and ESnet, so the unscheduled downtime on average is less than 10% of the total scheduled operating time. [Goal Met] | Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used was accounted for by computations that required at least 1/8 of the total resource. [Goal Not Met] | Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that was accounted for by computations that require at least 1/8 of the total resource. [Goal Met] | Focus usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that is accounted for by computations that require at least 1/8 of the total resource. FY 2006— 40% | Focus usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that is accounted for by computations that require at least 1/8 of the total resource. FY 2007— 40% |

## Means and Strategies

The ASCR program will use various means and strategies to achieve its goals. However, various external factors may impact the ability to achieve these goals.

ASCR will support fundamental, innovative, peer-reviewed research to create new knowledge in areas of advanced computing research that are important to DOE. In addition, ASCR will plan, fabricate, assemble, and operate premier supercomputer and networking facilities that serve researchers at national laboratories, universities, and industry, thus enabling new understanding through analysis, modeling, and simulation for complex problems, and effective integration of geographically distributed teams through national laboratories. Finally, the program will continue its leadership of the SC-wide SciDAC initiative with BES and BER in the areas of nanotechnology and Genomics: GTL. All research projects undergo regular peer review and merit evaluation based on procedures outlined in 10 CFR 605 for the extramural grant program, and under a similar process for the laboratory programs and scientific user facilities. All new projects are selected through peer review and merit evaluation.

External factors that affect the programs and performance include: (1) mission needs as described by the DOE and SC mission statements and strategic plans; (2) evolving scientific opportunities, which sometimes emerge in a way that revolutionizes disciplines; (3) results of external program reviews and international benchmarking activities of entire fields or subfields, such as those performed by the National Academy of Sciences (NAS); (4) unanticipated failures, e.g., in the evaluation of new computer architectures for science, that cannot be mitigated in a timely manner; (5) strategic and programmatic decisions made by other (non-DOE) Federal agencies and by international entities; and (6) the evolution of the commercial market for high performance computing and networking hardware and software.

The fundamental research program and facilities supported by ASCR are closely coordinated with the information technology research activities of other Federal Agencies (Defense Advanced Research Projects Administration [DARPA], Environmental Protection Agency [EPA], National Aeronautics and Space Administration [NASA], National Institute of Health [NIH], National Security Agency [NSA], and National Science Foundation [NSF]) through the Computing Information and Communications Research and Development (R&D) subcommittee of the National Science and Technology Council (NSTC), under the auspices of SC and Technology Policy. This coordination is periodically reviewed by the President's Information Technology Advisory Committee (PITAC). In addition to this interagency coordination, ASCR has a number of partnerships with other programs in SC and other parts of the Department, focused on advanced application testbeds to apply the results of ASCR research. Finally, ASCR has a significant ongoing coordination effort with the National Nuclear Security Administration's (NNSA) Advanced Science Computing (ASC) Campaign to ensure maximum effectiveness of both computational science research efforts.

## Validation and Verification

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

## Program Assessment Rating Tool (PART)

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

In FY 2005 PART review, OMB gave the ASCR program an overall rating of "Moderately Effective." OMB found that: the program supports a supercomputer user facility and targeted research programs in applied math, computer science, and computational application software, many of which have been historically regarded as world class and of high quality; and the program's performance measures focus on the extent to which unique, large simulations are efficiently enabled by its software development activities and supercomputer user facilities. However, OMB was concerned that the program's external advisory committee is underutilized. In addition, OMB found that the program supports world-class scientific user facilities, has demonstrated an improved level of interagency communication and cooperation, is in the process of drafting a long-term strategic vision, and has been very successful with a major effort in interdisciplinary software. The assessment found that ASCR has developed a limited number of adequate performance measures which are continued for FY 2007. These measures have been incorporated into this budget request, ASCR grant solicitations, and the performance plans of senior managers. As appropriate, they will be incorporated into the performance-based contracts of Management and Operating (M&O) contractors. To better explain these complex scientific measures, SC has developed a website (http://www.sc.doe.gov/measures/) that answers questions such as "What does this measure mean?" and "Why is it important?" Roadmaps, developed in consultation with the Advanced Scientific Computing Advisory Committee (ASCAC) and also available on the website, will guide reviews every three years by ASCAC of progress toward achieving the long-term Performance Measures. The Annual Performance Targets are tracked through the Department's Joule system and reported in the Department's Annual Performance Report. In response to PART findings, ASCR established a Committees of Visitors (COV) to provide outside expert validation of the program's merit-based review processes for impact on quality, relevance, and performance. ASCR has received the reports from the first COV, which focused on the research programs, and the second COV, which met April 5-6, 2005, to review the facilities and network research efforts, and is working on an action plan to respond to the recommendations. In order to address specific concerns ASCR has made plans in FY 2006 and future fiscal years to: engage advisory panel and other outside groups in regular, thorough scientific assessments of the quality, relevence, and performance of its research portfolio and computing/network facilities; engage advisory panel and other outside groups in assessments of the program's progress in achieving its long-term goals, and in studies that revisit the strategic priorities for the program; and to implement action plans to improve program management in response to past expert reviews.

For the FY 2007 Budget, OMB has developed PARTWeb – a new interface for PART that facilitates collaboration between agencies and OMB. PARTWeb will link to the website http://ExpectMore.gov and will improve public access to PART assessments and follow up actions. For 2006 there are three actions for Advanced Scientific Computing Research.

- Engaging advisory panel and other outside groups in regular, thorough scientific assessments of the quality, relevance, and performance of its research portfolio and computing/network facilities.
- Engaging advisory panel and other outside groups in assessments of the program's progress in achieving its long-term goals, and in studies that revisit the strategic priorities for the program.
- Implementing action plans for improving program management in response to past expert reviews.

In response, ASCR will charge the Advanced Scientific Computing Research Advisory Committee to review progress toward the long term goals of the program before the end of FY 2006 and will continue to host Committees of Visitors (CoV) and other panels to review the quality, relevance, and performance of the program. ASCR will continue to publish responses to the COV's findings and will track improvements at http://www.sc.doe.gov/measures/FY06.html.

### Overview

Computational modeling and simulation are among the most significant developments in the practice of scientific inquiry in the 20th Century. Scientific computing is particularly important for the solution of research problems that are insoluble by traditional theoretical and experimental approaches, hazardous to study in the laboratory, or time-consuming or expensive to solve by traditional means. All of the SC research programs—Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy Physics, and Nuclear Physics—have identified major scientific challenges that can only be addressed through advances in scientific computing.

ASCR research underpins the efforts of the other programs in SC. The applied mathematics research activity produces the fundamental mathematical methods to model complex physical and biological systems. The computer science research efforts enable scientists to efficiently perform scientific computations on the highest performance computers available and to store, manage, analyze, and visualize the massive amounts of data that result. The networking research activity provides the techniques to link the data producers (e.g., supercomputers and large experimental facilities) with scientists who need access to the data.

ASCR's other principal responsibility is to provide the high-performance computational and networking resources that are required for world leadership in science. Recent dramatic advances in scientific computation by researchers and computer companies underscore the importance of strengthening our position in computational sciences in strategic areas. The Administration has recognized the importance of high-end computing. As stated in the "Analytical Perspectives" of the FY 2004 Budget:

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

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

## How We Work

The ASCR program uses a variety of mechanisms for conducting, coordinating, and funding research in applied mathematics, network and computer sciences, and in advanced computing software tools. The program is responsible for planning and prioritizing all aspects of supported research, conducting ongoing assessments to ensure a comprehensive and balanced portfolio, regularly seeking advice from stakeholders, supporting core university and national laboratory programs, and maintaining a strong infrastructure to support research in applied mathematics, network and computer science, and advanced computing software tools. The quality of the research supported by the ASCR program is continuously evaluated through the use of merit-based peer review, scientific advisory committees, and interagency coordinating bodies.

### Advisory and Consultative Activities

The Advanced Scientific Computing Advisory Committee (ASCAC)—though inactive in 2005—provides valuable, independent advice to DOE on a variety of complex scientific and technical issues related to the ASCR program. The ASCAC is charged with providing advice on promising future directions for advanced scientific computing research; strategies to couple advanced scientific computing research to other disciplines; and the relationship of the DOE program to other Federal investments in information technology (IT) research. ASCAC's recommendations include advice on long-range plans, priorities, and strategies to address more effectively the scientific aspects of advanced scientific computing including the relationship of advanced scientific computing to other scientific disciplines, and maintaining appropriate balance among elements of the program. This advisory committee plays a key role in assessing the scientific and programmatic merit of presently funded activities and in evaluating plans for the future. The Committee formally reports to the SC Director and includes representatives from universities, national laboratories, and industries who are involved in advanced computing research. Particular attention is paid to obtaining a diverse membership with a balance among scientific disciplines, institutions, and geographic regions. ASCAC operates in accordance with the Federal Advisory Committee Act (FACA), Public Law 92–463; and all applicable FACA Amendments, Federal Regulations, and Executive Orders.

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

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

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

- DOE Science Computing Conference, June 2003 (http://www.doe-sci-comp.info);
- Science Case for Large Scale Simulation, June 2003;
- Workshop on the Road Map for the Revitalization of High End Computing (http://www.cra.org/Activities/workshops/nitrd/);
- Cyber Infrastructure Report (http://www.nsf.gov/publications/pub_summ.jsp?ods_key=cise051203);
- "Federal Plan for High-End Computing, report of the High End-Computing Revitalization Task Force (HECRTF)" (http://www.itrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf); and
- The Office of Science Data-Management Challenge, Report from the DOE Office of Science Data-Management Workshops (http://www.sc.doe.gov/ascr/Final-report-v26.pdf).

**Facility Operations Reviews**

The ASCR program has undertaken a series of operations reviews of the National Energy Research Scientific Computing Center (NERSC), the Energy Sciences Network (ESnet), the Advanced Computing Research Testbeds (ACRTs), and the Leadership Computing Facilities (LCFs).

NERSC, operated by the Lawrence Berkeley National Laboratory (LBNL), annually serves about 2,000 scientists throughout the United States as SC's high performance production computing facility. These researchers work at DOE laboratories, universities, industrial laboratories, and other Federal agencies. Allocations of computer time and archival storage at NERSC are awarded to research groups based on a review of submitted proposals. As proposals are submitted, they are subjected to peer review to evaluate the quality of science, the relevance of the proposed research to SC goals and objectives, and the readiness of the proposed application to fully utilize the computing resources being requested. ASCR conducted a formal cost and schedule review, adapting processes used to manage construction projects, in May 2005.

The ESnet, managed and operated by the LBNL, is a high-speed network serving thousands of DOE scientists and collaborators worldwide. A pioneer in providing DOE mission-oriented high-bandwidth, reliable connections, ESnet enables researchers at national laboratories, universities, and other institutions to communicate with each other using the leading edge collaborative capabilities, not available in the commercial world, that are needed to address some of the world's most important scientific challenges. The ESnet Steering Committee (ESSC) was established in 1985 to ensure that ESnet meets the needs of SC programs. All program offices in SC appoint a representative to serve on the ESSC. The ESSC is responsible for reviewing and prioritizing network requirements, for establishing performance objectives, and for proposing innovative techniques for enhancing ESnet capabilities. In addition to the ongoing oversight from the ESSC, ASCR conducts regular external peer reviews of ESnet performance. The last such review was chaired by a member of ASCAC and took place in September 2001. The next review is scheduled in 2006.

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

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

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

In FY 2004, ASCR conducted a peer review of the CCS evaluation of the Cray X1 computer. The results from this review validated the exceptionally effective results of the evaluation and its contributions to the Federal high performance computing effort. Also in FY 2004, ASCR conducted a peer reviewed competition to establish a Leadership Computing Facility (LCF) for Open Science. This competition was won by a partnership of ORNL's CCS with Argonne National Laboratory (ANL) and Pacific Northwest National Laboratory (PNNL) that located the first LCF at the CCS. In March 2005, the SC Project Assessment group conducted a formal Baseline validation review of the ORNL LCF.

**Program Reviews**

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

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

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

**Planning and Priority Setting**

The ASCR program must coordinate and prioritize a large number of goals from agency and interagency strategic plans. One of the most important activities of ASCAC is the development of a framework for the coordinated advancement and application of network and computer science and applied mathematics. This framework must be sufficiently flexible to rapidly respond to developments in a fast paced area of research. The key planning elements for this program are:

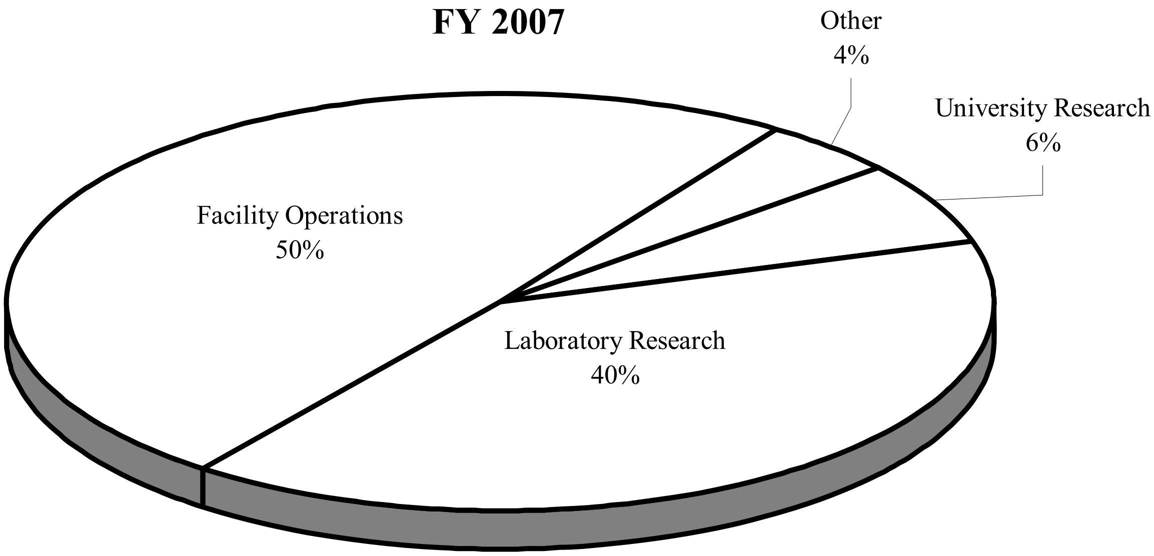
- The Department and SC Strategic Plan, as updated through program collaborations and joint advisory committee meetings (http://www.sc.doe.gov/Sub/Mission/mission_strategic.htm);
- SciDAC plan delivered to Congress in March 2000 (http://www.science.doe.gov/scidac/);
- ASCAC report on the Japanese Earth Simulator (http://www.sc.doe.gov/ascr/ascac_reports.htm); and
- The HECRTF Plan (http://www.itrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf).

**How We Spend Our Budget**

The ASCR program budget has one subprogram: Mathematical, Information and Computational Sciences (MICS). The MICS subprogram has two major components: research and facility operations.

The FY 2007 budget request continues the core and SciDAC research efforts and strengthens the research partnerships with other SC offices. Network operations expenditures account for 22% of the national laboratory research. The LTR subprogram was brought to a successful completion in FY 2004.

**Advanced Scientific Computing Research Budget Allocation FY 2007**




### Research

46 percent of the ASCR program's FY 2007 funding will be provided to scientists at universities and laboratories to conduct research. National laboratory research scientists work together with the other programs of SC to develop the tools and techniques that allow those programs to take advantage of terascale computing for scientific research. The laboratories provide state-of-the-art resources for testbeds and novel applications. The division of support between national laboratories and universities is adjusted to maximize scientific productivity.

- ***University Research***: University researchers play a critical role in the nation's research effort and in the training of graduate students. During FY 2005, the ASCR program supported over 150 grants to the nation's university researchers and graduate students engaged in civilian applied mathematics, large-scale network and computer science research. In addition, ASCR supports a Computational Science Graduate Fellowship (CSGF) and an Early Career Principal Investigator (ECPI) activity in Applied Mathematics, Computer Science and High-Performance Networks. In FY 2005, CSGF activity selected 15 new graduate students representing 12 universities and 8 states. Approximately half of those who received Ph.D.'s in the CSGF program between 1991 and 2001 are pursuing careers outside universities or national labs. ASCR also provides support to other SC research programs. The ECPI activity made 12 awards to early career principal investigators in FY 2005.

The university grants program is proposal driven, similar to the computer science and applied mathematics programs at the National Science Foundation (NSF). However, ASCR grant solicitation notices are focused on topics that have been identified as important for DOE missions. ASCR funds the best among the ideas submitted in response to grant solicitation notices (http://www.sc.doe.gov/grants/grants.html). Proposals are reviewed by external scientific peers and competitively awarded according to the guidelines published in 10 CFR 605 (http://www.science.doe.gov/production/grants/605index.html).

- ***National Laboratory Research***: ASCR supports national laboratory-based research groups at Argonne, Brookhaven, Los Alamos, Lawrence Berkeley, Lawrence Livermore, Oak Ridge, Pacific Northwest, and Sandia national laboratories and Ames Laboratory. The directions of laboratory research programs are driven by the needs of the Department and the unique capabilities of the laboratories to support large scale, multidisciplinary, collaborative research activities. In addition, laboratory-based research groups are highly tailored to the major scientific programs at the individual laboratories and the computational research needs of SC. Laboratory researchers collaborate with other laboratory and academic researchers, and are important for developing and maintaining testbeds and novel applications of high performance computing and networking in SC research. At Los Alamos, Livermore, and Sandia, ASCR funding plays an important role in supporting basic research that can improve programs, such as NNSA's Advanced Scientific Computing and Science-Based Stockpile Stewardship programs.

ASCR funds field work proposals from the national laboratories. Proposals are reviewed by external scientific peers and awarded using procedures that are equivalent to the 10 CFR 605 guidelines used for the grants program. Performance of the laboratory groups is reviewed by ASCR staff annually to examine the quality of their research and identify needed changes, corrective actions or redirection of effort. Individual laboratory groups have special capabilities or access to laboratory resources that can be profitably utilized in the development of the research program.

### Significant Program Shifts

The ASCR program advances mathematics and computer science, and develops the specialized algorithms, the scientific software tools, and the software libraries needed by DOE researchers to effectively use high-performance computing and networking hardware for scientific discovery. The ASCR program has been a leader in the computational sciences for several decades and has been acknowledged for pioneering accomplishments. The FY 2007 ASCR budget is focused in priority areas identified by the Joint Office of Management and Budget (OMB) and Office of Science and Technology Policy (OSTP) Research Priorities memorandum.

Major elements of the ASCR portfolio related to SciDAC are being recompeted in FY 2006, with attention paid to support for the long term maintenance and support of software tools such as mathematical libraries, adaptive mesh refinement software, and scientific data management tools developed in the first 5 years of the effort. In addition, in FY 2006 ASCR is changing the way in which it manages its Genomics: GTL partnership with BER. The management of these efforts will be integrated into the portfolio of successful SciDAC partnerships. Finally, in FY 2007 ASCR will continue funding the competitively selected SciDAC institutes which can become centers of excellence in high end computational science in areas that are critical to DOE missions.

For the past two decades SC, and the worldwide scientific community, have been harvesting their success in building and developing the Internet. This has enabled roughly a doubling in bandwidth every two years with no increase in cost. However, the demands of today's facilities, which generate millions of gigabytes per year of data, now outstrip the capabilities of the Internet design. The evolution of the telecom market, including the availability of direct access to optical fiber at attractive prices and the availability of flexible dense wave division multiplexing (DWDM) products gives SC the possibility of exploiting these technologies to provide scientific data where it is needed at speeds commensurate with the new data volumes. However, to take advantage of this opportunity significant research is needed to integrate these capabilities, make them available to scientists, and build the infrastructure which can provide cybersecurity in this environment.

The ORNL LCF, selected under the Leadership Computing Competition in FY 2004, will continue its evolution into a true leadership facility. The LCF as well as the enhancement of NERSC are aligned with the plan developed by the HECRTF established by the NSTC and OSTP. This area has been identified as a priority within the overall Networking and Information Technology Research and Development (NITR&D) priorities of the Administration. In prior budgets some, but not all, of the activities related to the HECRTF plan were described as components of the Next Generation Architecture (NGA) effort. We have eliminated discussion of the NGA to enable a clearer description of how ASCR research and facilities contribute to the HECRTF plan.

In FY 2007, further diversity with the LCF resources will be realized with an acquisition by ANL of a high performance IBM Blue Gene P with low-electrical power requirements and a peak capability of up to 100 teraflops. The expansion of the Leadership Computing Facility to include the Blue Gene computer at ANL was an important element of the joint ORNL, ANL, and PNNL proposal selected in 2004. This capability will accelerate scientific understanding in areas that include materials science, biology, and advanced designs of nuclear reactors.

These changes were made to guarantee the continued quality, relevance, and performance of ASCR programs. All ASCR activities undergo prospective and retrospective merit reviews and our extensive use of partnerships with other SC programs ensures the relevance of our efforts to SC missions.

**Interagency Environment**

The activities funded by the MICS subprogram are coordinated with other Federal efforts through the NITR&D subcommittee of the National Science and Technology Council and its Technology Committee. The NITR&D subcommittee evolved through an interagency coordination process that began under the 1991 High Performance Computing Act as the High Performance Computing, Communications, and Information Technology (HPCCIT) Committee. The NITR&D Subcommittee provides hands-on coordination for the multiagency NITR&D Program. The Subcommittee is made up of representatives from each of the participating NITR&D agencies and from the Office of Management and Budget (OMB), the NSTC, and the National Coordination Office for IT R&D (NCO/IT R&D). The Subcommittee coordinates planning, budgeting, and assessment activities of the multiagency NITR&D enterprise. DOE has been an active participant in these coordination groups and committees since their inception. The MICS subprogram will continue to coordinate its activities through these mechanisms and will lead the development of new coordinating mechanisms as needs arise. The DOE program solves mission critical problems in scientific computing. In addition, results from the DOE program benefit the Nation's information technology basic research effort. The FY 2007 program positions DOE to make additional contributions to this effort. In the area of high performance computing and computation, ASCR has extensive partnerships with other Federal agencies and the NNSA. Examples include: participating in the program review team for the DARPA High Productivity Computing Systems program; serving on the planning group for the Congressionally mandated DOD plan for high performance computing to serve the national security mission; serving on the OSTP High End Computing Revitalization Task Force; and extensive collaboration with NNSA-Advanced Simulation Computing. In FY 2003, ASCR formalized many of these interactions by developing a Memorandum of Understanding with SC, NNSA, DOD's Under Secretary for Defense Research and Engineering, DARPA, and the National Security Administration to coordinate research, development, testing, and evaluation of high performance computers.

### Scientific Discovery through Advanced Computing

The Scientific Discovery through Advanced Computing (SciDAC) program is a set of coordinated investments across all SC mission areas with the goal of achieving breakthrough scientific advances via computer simulation that were impossible using theoretical or laboratory studies alone. The power of computers and networks is increasing exponentially. Advances in high-end computing technology, together with innovative algorithms and software, are being exploited as intrinsic tools for scientific discovery. SciDAC has also pioneered an effective new model of multidisciplinary collaboration among discipline-specific scientists, computer scientists, computational scientists, and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can productively exploit terascale computing and networking resources. The program is bringing computation and simulation to parity with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate modeling and prediction, plasma physics, particle physics, accelerator design, astrophysics, chemically reacting flows, and computational nanoscience.

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

In FY 2006, ASCR is recompeting its SciDAC portfolio, with the exception of activities in partnership with the Office of Fusion Energy that were initiated in FY 2005. In addition, in FY 2007 ASCR will continue the competitively selected SciDAC institutes which can become centers of excellence in high end computational science in areas that are critical to DOE missions.

### Scientific Facilities Utilization

The ASCR program's FY 2007 request includes support to the NERSC, ESnet, and the LCFs, located at ORNL's CCS and ANL. The investment in NERSC will provide computer resources for about 2,000 scientists in universities, DOE laboratories, Federal agencies, and U.S. companies. The proposed funding will enable NERSC to maintain its role as one of the Nation's premier unclassified computing centers, a critical element for success of many SC research programs. The investment in ESnet will provide the DOE science community with capabilities not available through commercial networks or the commercial Internet. ESnet provides national and international high-speed access to DOE and SC researchers and research facilities, including light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, supercomputers, and other high impact scientific instruments. The investment in LCFs will deliver unclassified high performance capability resources to scientific researchers as described in the HECRTF report. The proposed funding will allow the high performance resources at the LCFs to be upgraded to a peak capability of 150 Teraflops in FY 2007.

| | FY 2005 | FY 2006 Estimate | FY 2007 Estimate |
|---|---|---|---|
| NERSC | | | |
| Maximum Hours | 8,760 | 8,760 | 8,760 |
| Scheduled Hours | 8,585 | 8,585 | 8,585 |
| Unscheduled Downtime | 1% | 1% | 1% |
| ESnet | | | |
| Maximum Hours | 8,760 | 8,760 | 8,760 |
| Scheduled Hours | 8,585 | 8,585 | 8,585 |
| Unscheduled Downtime | 1% | 1% | 1% |
| LCF-ORNL | | | |
| Maximum Hours | 7,008 | 7,008 | 7,008 |
| Scheduled Hours | 7,008 | 7,008 | 7,008 |
| Unscheduled Downtime | 1% | 1% | 1% |

## Workforce Development

The R&D Workforce Development mission is to ensure the supply of computational and computer science Ph.D. level scientists for the Department and the Nation through graduate student and postdoctoral research support. In FY 2007, this program will support approximately 800 graduate students and post doctoral investigators, of which 500 will be supported at SC user facilities.

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

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

# Mathematical, Information, and Computational Sciences

## Funding Schedule by Activity

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

### Description

The Mathematical, Information, and Computational Sciences (MICS) subprogram is responsible for carrying out the mission of the ASCR program: To deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.

### Benefits

MICS supports ASCR's contribution to DOE's mission to provide world-class scientific research capacity by providing world-class, peer-reviewed scientific results in mathematics, high performance computing and advanced networks and applying the potential of terascale computing to advanced scientific applications. Computer-based simulation enables us to predict the behavior of complex systems that are beyond the reach of our most powerful experimental probes or our most sophisticated theories. Computational modeling has greatly advanced our understanding of fundamental processes of nature, such as fluid flow and turbulence or molecular structure and reactivity. Through modeling and simulation, we will be able to explore the interior of stars and learn how protein machines work inside living cells. We can design novel catalysts and high-efficiency engines. Computational science is increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering. The science of the future demands that we advance beyond our current computational abilities. Accordingly, we must address the following questions:

- What new mathematics are required to effectively model systems such as the earth's climate or the behavior of living cells that involve processes taking place on vastly different time and/or length scales?
- Which computational architectures and platforms will deliver the most benefit for the science of today and the science of the future?
- What advances in computer science and algorithms are needed to increase the efficiency with which supercomputers solve problems for SC?
- What operating systems, data management, analysis, model development, and other tools are required to make effective use of future-generation supercomputers?

- Is it possible to overcome the geographical distances that often hinder science by making all scientific resources readily available to scientists, regardless of whether they are at a university, national laboratory, or industrial setting?

To answer these questions and develop the algorithms software and tools that are needed, MICS has developed four strategies (the strategy numbers refer to the SC Strategic Plan):

6.1 Advance scientific discovery through research in the computer science and applied mathematics required to enable prediction and understanding of complex systems.

6.2 Extend the frontiers of scientific simulation through a new generation of computational models that fully exploit the power of advanced computers and collaboratory software that makes scientific resources available to scientists anywhere, anytime.

6.3 Bring dramatic advances to scientific computing challenges by supporting the development, evaluation, and application of supercomputing architectures tailored to science.

6.4 Provide computing resources at the petascale and beyond, network infrastructure, and tools to enable computational science and scientific collaboration.

All MICS investments directly contribute to one or more of these strategies.

**Supporting Information**

Discussions of the extent to which the requirements of the Office of Science exceed current capabilities and capacity can be found in a number of reports including: "Federal Plan for High-End Computing, Report of the High-End Computing Revitalization Task Force (HECRTF)" May 10, 2004, Appendices A-1, A-2, and A-3, (http://www.sc.doe.gov/ascr/hecrtfrpt.pdf); "A Science-Based Case for Large-Scale Simulation," Volume 1, July 30, 2003, (http://www.sc.doe.gov/ascr/Scalesreptvol1.pdf); "Theory and Modeling in Nanoscience, Report of the May 10-11, 2002 Workshop conducted by the Basic Energy Sciences and Advanced Scientific Computing Advisory Committees to SC, Dept. of Energy," (http://www.sc.doe.gov/ascr/TMN_rpt.pdf); "Integrated Simulation and Optimization of Magnetic Fusion Systems, Report of the FESAC Panel," November 2, 2002, (http://www.ofes.fusion.doe.gov/News/FSP_report_Dec9.pdf); and "High-Performance Networks for High-Impact Science, Report of the High-Performance Network Planning Workshop conducted August 13-15, 2002," (http://www.sc.doe.gov/ascr/high-performance_networks.pdf). Furthermore, the algorithms and software tools, libraries, and environments needed to accelerate scientific discovery through modeling and simulation are beyond the realm of commercial interest. To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, the MICS subprogram employs a broad, but integrated, research strategy. The MICS subprogram's basic research portfolio in applied mathematics and computer science provides the foundation for enabling research activities, which includes efforts to advance networking and to develop software tools, libraries, and environments. Results from enabling research supported by the MICS subprogram are used by computational scientists supported by other SC and DOE programs. This link to other DOE programs provides a tangible assessment of the value of the MICS subprogram for advancing scientific discovery and technology development through simulations.

In addition to its research activities, the MICS subprogram plans, develops, and operates supercomputer and network facilities that are available—24 hours a day, 365 days a year—to researchers working on problems relevant to DOE's scientific missions.

The Early Career Principal Investigator (ECPI) activity was initiated in FY 2002 for scientists and engineers in tenure track positions at U.S. universities. Seventeen awards were made in FY 2002, twelve awards in FY 2003, sixteen in FY 2004, and twelve in FY 2005. Additional awards will be made in FY 2006 for this activity, pending the outcome of review of applications. The goal of the ECPI activity is to support SC mission-related research in applied mathematics, computer science, and high-performance networks performed by exceptionally talented university investigators, who are at an early stage in their professional careers.

**FY 2005 Accomplishments**

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

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

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

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

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

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

**FY 2005 Awards**

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

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

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

## Detailed Justification

(dollars in thousands)

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| **Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research** | **108,105** | **105,275** | **117,122** |
| ▪ **Applied Mathematics** | **29,577** | **29,354** | **29,495** |

This activity supports research on the underlying mathematical understanding of physical, chemical, and biological systems, and on advanced numerical algorithms that enable effective description, modeling, and simulation of such systems on high-end computing systems. It directly supports SC Strategic Plan strategy 6.1. Research in Applied Mathematics supported by the MICS subprogram underpins computational science throughout DOE. Historically, the numerical algorithms developed under this activity have produced scientific advances through simulation that are as significant as those resulting from improvements in computer hardware. This activity supports research at DOE laboratories, universities, and private companies. Many of the projects supported by this activity involve research partnerships between DOE's national laboratories and universities. The activity supports research in a wide variety of areas of mathematics, including: ordinary and partial differential equations and solution methods, including techniques to convert equations into discrete elements and boundary integral methods; advanced treatment of interfaces and boundaries (fast marching and level set methods, and front tracking); numerical linear algebra (advanced iterative methods, general and problem-specific preconditioners, sparse solvers, and dense solvers); fluid dynamics (compressible, incompressible, and reacting flows, turbulence modeling, and multiphase flows); optimization (linear and nonlinear programming, interior-point methods, and discrete and integer programming); mathematical physics; control theory (differential-algebraic systems, order reduction, and queuing theory); accurate treatment of shock waves; "fast" methods (fast multipole and fast wavelet transforms); mixed elliptic-hyperbolic systems; dynamical systems (chaos theory, optimal control theory, and bifurcation theory); automated reasoning systems; and multiscale mathematics. This final area represents our most recent effort at focusing on those mission-related applications which span wide ranges of interacting length- and time-scales.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

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

| | | | |
|---|---|---|---|
| ▪ **Computer Science** | **21,590** | **24,271** | **23,863** |

This activity supports research in computer science to enable computational scientists to effectively utilize high-performance computers to advance science in areas important to the DOE mission. This activity supports SC Strategic Plan strategies 6.1 and 6.3. DOE has unique requirements for high performance computing that significantly exceed the capability of software products from computer vendors. This activity supports computer science research in two general areas: the underlying software to enable applications to make effective use of computers with hundreds or thousands of processors as well as computers that are located at different sites; and large scale data management and visualization for both local data analysis and for circumstances where key resources and users are geographically distributed. Research areas include: tools to monitor the performance of scientific applications and enable users to improve performance and get scientific results faster; new programming models to simplify application code development; advanced techniques for visualizing very large-scale scientific data; and efforts to improve application performance through innovative next generation operating systems. Researchers at DOE laboratories and universities, often working in partnerships, propose and conduct this research.

All of the computer science research funded by this activity is reported to and coordinated through the High End Computing Interagency Working Group of the NITR&D Subcommittee. The quality, relevance, and performance of the program is continually monitored through extensive peer review, interagency reporting and coordination, and interaction with end users to assist in the determination of impact and future research priorities.

Beginning in FY 2004, this activity incorporated the software research component of the implementation of the HECRTF plan to improve application performance and system reliability through innovative approaches to next generation operating systems. This activity is coordinated with other agencies through the High End Computing University Research Activity (HEC URA), an outgrowth of the HECRTF. These activities will be modestly increased in FY 2007, especially in areas such as performance analysis of innovative high-end architectures; frameworks for data intensive and visual computing; intelligent program development environments; application-specific problem solving environments; and common compile and runtime infrastructures and interfaces, where ASCR is the leader in the Federal agency research efforts. This research will play a key role in the interagency strategy for high end software development.

| | | | |
|---|---|---|---|
| ▪ **Computational Partnerships** | **35,769** | **38,052** | **50,000** |

This activity supports the amalgam of those activities previously titled "Advanced Computing Software Tools" and "Scientific Applications Partnerships." The advanced computing software tools part of this activity supports research and development activities that extend key results from applied mathematics and computer science research to develop integrated software tools that computational scientists can use in high performance scientific applications (such as characterizing and predicting phase changes in materials). These tools, which enable improved performance on high-end systems, are critical to the ability of scientists to attack the complex scientific and engineering problems that can only be solved with such systems. This activity directly supports SC Strategic Plan strategy 6.2.

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

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

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

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

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

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

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

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

This activity builds the understanding that will enable ESnet as well as other Research and Education Networks such as the Internet2 Abilene network to fully take advantage of the opportunity to make optical networks tools for science. In much the same way that early scientific use of the Internet enabled today's worldwide infrastructure, the experience of scientists on these new optical networks is expected to influence the next generation of high performance networks for the country. For example, it includes standards-based network protocols and middleware that address challenging issues such as security, information location, and network performance that are encountered with ultra-high-speed data transfers, remote visualization, real-time remote instrumentation, and large-scale scientific collaboration. These tools provide a new way of organizing and performing scientific work, e.g., distributed teams and real-time remote access to SC facilities that offers the potential for increased productivity and efficiency. It will also enable broader access to important DOE facilities and data resources by scientists and educators throughout the country. It is particularly important to

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

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

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

This activity directly supports SC Strategic Plan strategy 6.4 through a portfolio of capabilities that range from Research and Evaluation Prototypes (R&E Prototypes) to Leadership Class Computers (LCCs) to High Performance Production Computing (HPPC). This activity integrates activities previously described separately as NERSC and ACRTs. It includes NERSC and resources at the ORNL Center for Computational Sciences (CCS). Related requirements for capital equipment, such as high-speed disk storage systems, archival data storage systems, and high performance visualization hardware are also supported. FY 2007 capital equipment requirements for these types of capital equipment are increased from FY 2006.

| | | | |
|---|---|---|---|
| • **High Performance Production Computing** | **37,868** | **37,489** | **54,790** |

This activity supports the National Energy Research Scientific Computing Center (NERSC), located at the LBNL. NERSC delivers high-end capacity computing services and support to the entire DOE SC research community and provides the majority of resources and services that are used to support SC SciDAC programs. The center serves 2,000 users working on about 700 projects. 35% of users are university based, 61% are in National Laboratories, 3% are in industry, and 1% are in other government laboratories. FY 2007 funding will support the continued operation of NERSC 3e at 10 teraflops peak performance, and the computer systems, NCSa and NCSb, with a combined peak performance of 10 teraflops. NCSa and NCSb are focused on high performance production computing for scientific applications that do not scale well to more than 512 processors and are not well suited to the NERSC 3e. In addition, in FY 2006, a procurement is planned for the next generation of high performance resources at NERSC to be delivered in early FY 2007. The resultant NERSC-5 peak capacity is expected to be 100–150 teraflops by the end of FY 2007. These computational resources are integrated by a common high performance file storage system that enables users to easily use all the resources. The FY 2006 oversubscription at NERSC is about a factor of 6-8. In FY 2007, we will increase the capacity by about a factor of 6.

NERSC plays a key role in the SC strategy for computational science because it enables teams to prepare to make the best use of the Leadership Computing Facilities (LCF) as well as to perform the calculations that are required by the missions of SC.

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

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

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|

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

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▸ **Leadership Computing Facility at ORNL** | **48,600** | **53,702** | **80,000** |

The first LCF capability for science was established in late FY 2005 at ORNL with the acquisition of a Cray X1E, the most capable system available to scientific users in the U.S., and a complementary Cray Red Storm (XT3) system.

In FY 2007, the ORNL LCF will provide world leading high performance sustained capability to researchers on a peer-reviewed basis. The LCF will upgrade computers acquired in FY 2004 and FY 2005 to provide more than 250 teraflops peak capability by the end of FY 2007. These advancements will enable scientific advancements such as simulations of diesel combustion including realistic diesel fuel chemistry to minimize the processes that generate $NO_x$ and soot, simulations of fusion devices that approach ITER scale devices and quantum Monte Carlo calculations of complex chemical reactions that extend over experimentally relevant times. The success of this effort is built on the enhancements to the research and evaluation prototype and computer science research activities elsewhere.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▸ **Leadership Computing Facility at ANL** | — | — | **22,504** |

In FY 2007, further diversity with the LCF resources will be realized with an acquisition by ANL of a high performance IBM Blue Gene P with low-electrical power requirements and a peak capability of up to 100 teraflops. The expansion of the Leadership Computing Facility to include the Blue Gene computer at ANL was an important element of the joint ORNL, ANL, and PNNL proposal selected in 2004. This capability will accelerate scientific understanding in areas that include materials science, catalysis, protein/DNA complexes, and advanced designs of nuclear reactors. The IBM Blue Gene architecture is expected to deliver significantly greater performance per dollar for this class of applications than the computing at ORNL.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| • **Research and Evaluation Prototypes** | **13,028** | **12,959** | **13,000** |

The Research and Evaluation Prototype computer activity will prepare users for the next generations of scientific computers and reduce the risk of major procurements. This activity will be carried out in close partnership with the NNSA and the DARPA HPCS program. This effort is critical to address the challenges of the systems that will be available by the end of the decade. These systems will be ten times larger than those of today. Many of the issues that need to be addressed are shared with the computer science research effort described above.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **High Performance Network Facilities and Testbeds** | **18,579** | **18,966** | **22,736** |

This activity supports SC strategy to provide high capability networking services to support leading edge scientific research. This strategy integrates ESnet, a Wide Area Network (WAN) project that supports the scientific research mission of the DOE with a number of smaller Metropolitan Area Networks (MANs) that provide high bandwidth access to the ESnet backbone. The ESnet

(dollars in thousands)

| FY 2005 | FY 2006 | FY 2007 |
|---|---|---|

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

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

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

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

| | | | |
|---|---|---|---|
| **Total, Mathematical, Information, and Computational Sciences** | **226,180** | **234,684** | **318,654** |

## Explanation of Funding Changes

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

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

# Capital Operating Expenses and Construction Summary

## Capital Operating Expenses

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

# Biological and Environmental Research

## Funding Profile by Subprogram

| | (dollars in thousands) | | | | |
|---|---|---|---|---|---|
| | FY 2005 Current Appropriation | FY 2006 Original Appropriation | FY 2006 Adjustments | FY 2006 Current Appropriation | FY 2007 Request |
| Biological and Environmental Research | | | | | |
| Life Sciences | 198,643 | 204,035 | -2,040[a] | 201,995 | 264,158 |
| Climate Change Research | 135,535 | 142,959 | -1,430[a] | 141,529 | 134,909 |
| Environmental Remediation | 100,575 | 94,694 | -950[a] | 93,744 | 97,196 |
| Medical Applications and Measurement Science | 121,924 | 144,000 | -1,437[a] | 142,563 | 14,000 |
| Subtotal, Biological and Environmental Research | 556,677 | 585,688 | -5,857 | 579,831 | 510,263 |
| Construction | 9,920 | — | — | — | — |
| Total, Biological and Environmental Research | 566,597[b] | 585,688 | -5,857 | 579,831 | 510,263 |

**Public Law Authorization:**
Public Law 95-91, "Department of Energy Organization Act"
Public Law 109-58, "Energy Policy Act of 2005"

### Mission

The mission of the Biological and Environmental Research (BER) program is to advance environmental and biomedical knowledge that promotes national security through improved energy production, development, and use; international scientific leadership that underpins our Nation's technological advances; knowledge needed to support the President's National Energy Plan; and research that improves the quality of life for all Americans. BER supports these vital national missions through competitive and peer-reviewed research at national laboratories, universities, and private institutions.

### Benefits

BER supports DOE's mission of protecting our national and economic security by providing world-class scientific research capacity and advancing scientific knowledge by supporting world-class, peer-reviewed scientific results in biology and environmental science whose results are published in the scientific literature. Basic biological and environmental research has broad impacts on our health, our environment, and our energy future. An ability to predict long-range and regional climate enables effective planning for future needs in energy, agriculture, and land and water use. Biotechnology solutions are possible for DOE energy, environmental, and national security challenges by understanding complex biological systems and developing computational tools to model and predict their behavior. Understanding the global carbon cycle and the associated role and capabilities of microbes and plants

[a] Reflects a rescission in accordance with P.L. 109-148, the Emergency Supplemental Appropriations Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006.
[b] Total is reduced by $4,678,000 for a rescission in accordance with P.L. 108-447, the Consolidated Appropriations Act, 2005; $13,674,000, which was transferred to the SBIR program; and $1,641,000, which was transferred to the STTR program.

can lead to solutions for reducing carbon dioxide concentrations in the atmosphere. Understanding the complex role of biology, geochemistry, and hydrology beneath the Earth's surface will lead to improved decision making and solutions for contaminated DOE weapons sites. Both normal and abnormal health—from normal human development to cancer to brain function—can be understood and improved using radiotracers, advanced imaging instruments, and novel biomedical devices. Understanding the biological effects of low doses of radiation can lead to the development of science-based health risk policy to better protect workers and citizens.

**Strategic and Program Goals**

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

Science Strategic Goal
General Goal 5, World-Class Scientific Research Capacity: Provide world-class scientific research capacity needed to: ensure the success of Department missions in national and energy security; advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences; or provide world-class research facilities for the Nation's science enterprise.
The BER program has one program goal which contributes to General Goal 5 in the "goal cascade":
Program Goal 05.21.00.00: Harness the Power of Our Living World – Provide the biological and environmental discoveries necessary to clean and protect our environment, offer new energy alternatives, and facilitate the entrainment of physical sciences advances in the biomedical field.

**Contribution to Program Goal 05.21.00.00 (Harness the Power of Our Living World)**
BER contributes to Program Goal 05.21.00.00 by advancing fundamental research in climate change, environmental remediation, genomics, proteomics, radiation biology, and medical applications. BER supports leading research programs that provide world-class, merit-reviewed research results. Discoveries at these scientific frontiers will bring revolutionary and unconventional solutions to some of our most pressing and expensive challenges in energy and the environment.

We will understand how living organisms interact with and respond to their environments to be able to use biology to produce clean energy, remove excess carbon dioxide from the atmosphere, and help clean up the environment. Our understanding of global climate change and our ability to predict climate over decades to centuries will enable us to develop science-based solutions to minimize the impacts of climate change and to better plan for our Nation's future energy needs. Understanding the biological effects of low doses of radiation will lead to the development of science-based health risk policy to better protect workers and citizens. Understanding the fate and transport of environmental contaminants will lead the way to discovering innovative approaches for cleaning up the environment.

BER research leads to the development of advanced medical imaging technology, including radiopharmaceuticals for imaging to be used for diagnosis and treatment of disease. BER research also advances the development of a broad range of intelligent biomimetic electronics that can both sense and correctly stimulate the nervous system, e.g., an artificial retina that will enable the blind to see, and that will lead to development of intelligent micro machines that interface with the brain and spinal cord to overcome disabilities. This research capitalizes on the national laboratories' unique resources and expertise in biological, chemical, physical, and computational sciences for technological advances related to human health, and on their sophisticated instrumentation (neutron and light sources, mass spectroscopy, and high field magnets), lasers and supercomputers. This research is coordinated with other complementary Federal programs.

In addition, BER plans, constructs, and operates reliable, world-class scientific facilities to serve thousands of researchers at universities, national laboratories, and private institutions from all over the world. Activities include structural biology research beam lines at the synchrotron light sources and neutron sources; the operation of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) (including the Molecular Sciences Computing Facility) where research activities underpin long-term environmental remediation and other DOE missions in energy and national security; the Production Genomics Facility (PGF); the Laboratory for Comparative and Functional Genomics ("Mouse House"); and the climate change research facilities – the Atmospheric Radiation Measurement (ARM) and the Free-Air Carbon Dioxide Enrichment (FACE) facilities.

The following indicators establish specific long-term goals in Scientific Advancement that the BER program is committed to, and progress can be measured against.

- **Life Sciences:** Characterize the multi-protein complexes (or the lack thereof) involving a scientifically significant fraction of a microbe's proteins. Develop computational models to direct the use and design of microbial communities to clean up waste, sequester carbon, or produce hydrogen.
- **Climate Change Research:** Deliver improved climate data and models for policy makers to determine safe levels of greenhouse gases for the earth's system. By 2013, substantially reduce differences between observed temperature and model simulations at subcontinental scales using several decades of recent data.
- **Environmental Remediation:** By 2015, provide sufficient scientific understanding to allow a significant fraction of DOE sites to incorporate coupled biological, chemical and physical processes for decision making for environmental remediation and long-term stewardship.
- **Medical Applications and Measurement Science:** Develop intelligent biomimetic electronics that can both sense and correctly stimulate the nervous system.[a]
- **Facilities:** Manage facilities operations to the highest standards of overall performance using merit evaluation with independent peer review.

## Funding by General and Program Goal

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| General Goal 5, World-Class Scientific Research Capacity | | | |
| Program Goal 05.21.00.00 Harness the Power of Our Living World (Biological and Environmental Research)....... | 566,597 | 579,831 | 510,263 |

[a] This indicator is not a PART measure.

## Annual Performance Results and Targets

| FY 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Program Goal 05.21.00.00 (Harness the Power of Our Living World) | | | | | |
| Life Sciences | | | | | |
| Increase the rate of DNA sequencing; Produce at least 12.7 billion base pairs of high quality DNA microbial and model organism genome sequence. [Met Goal] | Increase the rate of DNA sequencing: Produce at least 14 billion base pairs of high quality DNA microbial and model organism genome sequence. [Met Goal] | Increase the rate of DNA sequencing: Produce at least 20 billion base pairs of high quality DNA microbial and model organism genome sequence. [Met Goal] | Increase the rate of DNA sequencing: Number (in billions) of base pairs of high quality (less than one error in 10,000 bases) DNA microbial and model organism genome sequence produced annually. FY 2005 at least 28 billion base pairs will be sequenced. [Met Goal] | Increase the rate of DNA sequencing: Number (in billions) of base pairs of high quality (less than one error in 10,000 bases) DNA microbial and model organism genome sequence produced annually. FY 2006 at least 30 billion base pairs will be sequenced. | Increase the rate and decrease the cost of DNA sequencing – Cost reductions will increase the number of high quality base pairs determined (less than one error in 10,000 bases) by 25% from the FY 2006 target of 582 base pairs per dollar to 781 base pairs per dollar. |
| Climate Change Research | | | | | |
| Improve climate models: Released a new coupled climate model with a horizontal resolution of 2.8 degrees (longitude and latitude) in the atmosphere and 0.7 degrees in the ocean and sea ice components, compared to the previous version with a resolution of 2.8 degrees in the atmosphere and 2.0 degrees in the ocean. Executed an 800-year equilibrium climate simulation with the new model. [Met Goal] | Improve climate models: Constructed a climate model for the next round of IPCC Working Group 1 Assessment simulations. This model increased the realism of the coupled atmosphere-ocean-land surface-sea ice system through improvements in the physical parameterizations, particularly the cloud sub models. The standard model increased the horizontal resolution to 1.4 degrees in the atmosphere and maintained the 0.7 degree resolution in the ocean and sea ice components. More objective and systematic methods to test (evaluate) the performance of both the model components (i.e., atmosphere, ocean, land surface, and sea ice sub models) as well as the fully coupled model, were applied. [Met Goal] | Improve climate models: Implement a model test bed system to incorporate climate data rapidly into climate models to allow testing of the performance of sub-models (e.g. cloud resolving module) and model parameters by comparing model simulations with real world data from the ARM sites and satellites. [Met Goal] | Improve climate models: Implement three separate component submodels (an interactive carbon cycle submodel, a secondary sulfur aerosol submodel, and an interactive terrestrial biosphere submodel) within a climate model and conduct 3-4 year duration climate simulation using the fully coupled model. [Met Goal] | Improve climate models: Produce a new continuous time series of retrieved cloud properties at each ARM site and evaluate the extent of agreement between climate model simulations of water vapor concentration and cloud properties and measurements of these quantities on the timescale of 1 to 4 days | Provide new mixed-phase cloud parameterization for incorporation in atmospheric GCMs and evaluate extent of agreement between climate model simulations and observations for cloud properties in the arctic. |

| FY 2002 Results | FY 2003 Results | FY 2004 Results | FY 2005 Results | FY 2006 Targets | FY 2007 Targets |
|---|---|---|---|---|---|
| Environmental Remediation | | | | | |
| Determine scalability of laboratory results in field environments: Using genomic sequencing data of key bioremediation microbes, such as Geobacter, Deinococcus, and Shewanella, determined that common soil microbes produce organic compounds that interact with radionuclides, such as plutonium, providing the molecular understanding for the detection and transformation of radionuclides in subsurface environments. [Met Goal] | Determine scalability of laboratory results in field environments: Identified naturally occurring microbial populations responsible for transformation of metals and radionuclides at DOE contaminated sites. [Met Goal] | Perform combined field/laboratory/modeling to determine how to interpret data at widely differing scales: Quantify contaminant immobilization and remobilization by different factors: 1. natural microbial mechanisms; 2. chemical reactions with minerals; and 3. colloid formation. [Met Goal] | Determine scalability of laboratory results in field experiments - Conduct two sets of field experiments to evaluate biological reduction of chromium and uranium by microorganisms and compare the results to laboratory studies to understand the long term fate and transport of these elements in field settings. [Met Goal] | Develop predictive model for contaminant transport that incorporates complex biology, hydrology, and chemistry of the subsurface. Validate model through field tests. | Implement a field-oriented, integrated experimental research program to quantify coupled processes that control reactive transport of at least one key DOE contaminant. |
| Medical Applications and Measurement Science[a] | | | | | |
| Advance blind patient sight: Developed technology to micromachine new flexible biocompatible material to be used as a platform for multi-electrode array artificial retina. [Met Goal] | Advance blind patient sight: Developed and tested materials for platform and sealants for a prototype artificial retina- a microelectronic array to be used for the treatment of blindness. [Met Goal] | Advance blind patient sight: Complete fabrication of 60 microelectrode array for use as an artificial retina and tested in animal subject. [Met Goal] | Advance blind patient sight: Complete testing on a 60 microelectrode array artificial retina and insert prototype device into a blind patient. [Met Goal] | Advance blind patient sight: Begin testing of prototypes for 256 microelectrode array artificial retina. | Advanced blind patient sight: complete design and construction of final 256 electrode array. Begin in vitro testing and non-stimulating testing in animals. |
| All BER Facilities | | | | | |
| Maintain and operate BER facilities such that achieved operation time is on average greater than 90% of the total scheduled annual operation time. [Met Goal] | Maintain and operate BER facilities such that achieved operation time is on average greater than 90% of the total scheduled annual operation time. [Met Goal] | Maintain and operate BER facilities such that achieved operation time is on average greater than 90% of the total scheduled annual operation time. [Met Goal] | Maintain and operate BER facilities (Life Science – PGF and the Mouse facility; Climate Change Research – ARM and FACE; and Environmental Remediation – EMSL) such that achieved operation time is on average greater than 90% of the total scheduled annual operation time for each group of facilities. [Met Goal] | Maintain and operate BER facilities (Life Science – PGF and the Mouse facility; Climate Change Research – ARM and FACE; and Environmental Remediation – EMSL) such that achieved operation time is on average greater than 95% of the total scheduled annual operation time for each group of facilities. | Maintain and operate BER facilities (Life Science – PGF and the Mouse facility; Climate Change Research – ARM and FACE; and Environmental Remediation – EMSL) such that achieved operation time is on average greater than 98% of the total scheduled annual operation time for each group of facilities. |

[a] This is not a PART measure.

## Means and Strategies

The BER program will use various means and strategies to achieve its program goals. However, various external factors may impact the ability to achieve these goals.

The BER program will continue its investments in core fundamental science and technologies needed to address the interfaces between scientific disciplines such as biology, physics, chemistry, engineering, and information science. Of highest priority will be the development of a new research infrastructure needed to understand fundamental biological principles underlying the function and control of biological systems, the heart of the Genomics: GTL program. This new research infrastructure of well-integrated, interdisciplinary research teams will form the basis of a new approach for studying complex biological systems and for using those systems to solve critical problems in energy and environmental cleanup.

Our ability to predict climate on global and regional scales and to develop strategies for the removal of excess carbon dioxide, suspected to adversely impact global climate, from the atmosphere will depend on the continued development of novel research tools and a close integration of experimental and computational research.

BER also plays a key role in constructing and operating a wide array of biological and environmental user facilities for the Nation's researchers, such as the Environmental Molecular Sciences Laboratory (EMSL), the Production Genomics facility, the Laboratory for Functional and Comparative Genomics, Atmospheric Radiation Measurement (ARM) facilities, and Free Air Carbon Dioxide Enrichment (FACE) facilities.

All BER-supported research projects undergo regular peer review and merit evaluation based on procedures set down in 10 CFR 605 for the extramural grant program, and under a similar process for the laboratory programs and scientific user facilities. All new projects are selected through peer review and merit evaluation.

External factors that affect the programs and performance include: (1) mission needs as described by the DOE and SC mission statements and strategic plans; (2) evolving scientific opportunities that sometimes emerge in ways that revolutionize disciplines; (3) results of external program reviews and international benchmarking activities of entire fields or subfields, such as those performed by the National Academies of Science; (4) unanticipated failures, for example, in critical components of scientific user facilities that cannot be mitigated in a timely manner; and (5) strategic and programmatic decisions made by other (non-DOE) Federal agencies and by international entities.

The BER program is closely coordinated with the activities of other federal agencies (e.g., National Institutes of Health [NIH], National Science Foundation [NSF], National Aeronautics and Space Administration [NASA], Department of Commerce/National Oceanic and Atmospheric Administration [NOAA], Environmental Protection Administration [EPA], Department of Agriculture [USDA], and Department of Defense [DOD]). BER Climate Change Research is coordinated with the U.S. Global Change Research Program, an interagency program codified by Public Law 101-606 and involving thirteen federal agencies and departments.

BER also promotes the transfer of the results of its basic research to contribute to DOE missions in areas of future energy sources, improved use of fossil fuels (carbon sequestration), reduced environmental impacts of energy production and use, and environmental cleanup.

## Validation and Verification

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

**Program Assessment Rating Tool (PART) Assessment**

The Department implemented a tool to evaluate selected programs. PART was developed by OMB to provide a standardized way to assess the effectiveness of the Federal Government's portfolio of programs. The structured framework of the PART provides a means through which programs can assess their activities differently than through traditional reviews. The Biological and Environmental Research Program has incorporated feedback from OMB into the FY 2007 Budget Request and has taken or will take the necessary steps to continue to improve performance.

The Biological and Environmental Research (BER) Program last completed PART in support of the FY 2005 Budget Request. At that time, the program was rated as "Effective."

In the FY 2004 PART, OMB recommended that BER form Committees of Visitors (COVs) to review management of the BER research portfolio. The FY 2005 PART Summary Sheet Recommended that the Department develop an appropriate action plan in response to the findings and recommendations of the Committee of Visitors within 30 days of receipt of the report. Two BER COVs have been formed. The first COV was charged on July 23, 2003, to look at the Climate Change Research Division. This COV met on March 1–3, 2004, and reported to the Biological and Environmental Research Advisory Committee (BERAC) in November 2004. The Department responded to this report in December 2004. The Second COV was charged on April 21, 2004, to look at the Environmental Remediation Sciences Division. This COV met on October 5–7, 2004, and reported to BERAC in November 2004. The Department responded to this report in December 2004. In the FY 2006 PART Summary Sheet, OMB found the timely BER responses to both reports to be thoughtful and thorough.

For the FY 2004 PART, BER worked with OMB to develop more meaningful long-term performance goals for the program. BER then worked with BERAC to ensure that these measures were ambitious yet realistic and to define for each what would be required for the program to be "successful" and "minimally effective". The FY 2005 PART Summary Sheet Recommended that the Department work with its advisory committee to develop research milestones against which future outside panels may judge interim progress toward achieving the long-term goals of the program. In the FY 2006 PART Summary Sheet, OMB found that the BER program's research milestones—as expressed in the new DOE program plans—were produced and reflect the strategic goals of the program, and the BER advisory committee as a whole has provided formal comments on the milestones. Panels will be charged to review progress toward the BER long-term goals using the criteria developed by BERAC and will report to the program in FY 2006.

For the FY 2007 Budget, OMB has developed PARTWeb—a new interface for PART that facilitates collaboration between agencies and OMB. PARTWeb will link to the http://ExpectMore.gov website and will improve public access to PART assessments and follow up actions. For 2006 there are three actions for Biological and Environmental Research.

- Engaging the National Academies in an independent assessment of the scientific basis and business case for the program's microbial genomics research efforts.
- Implementing the recommendations of past external panel reviews of the program's research portfolio and management practices.

- Reviewing operations of user facilities, and improving discrimination in identifying open user facilities versus collaborative research facilities.

In response, BER has engaged the National Academies to review Genomics: GTL and expects a report by February 12, 2006. BER will also continue to publish responses to the COV's findings and will track improvements at http://www.sc.doe.gov/measures/FY06.html. The Biological and Environmental Research Advisory Committee has been reviewing the user facilities. BER will act on the results of these reviews to improve facility management.

**Overview**

BER supports fundamental research in genomics, proteomics, radiation biology, climate change, environmental remediation, and medical sciences. BER supports leading edge research facilities used by public and private sector scientists across the range of BER disciplines. BER works with other federal agencies to coordinate research across all of its programs. BER validates its long-range goals through its advisory committee, the Biological and Environmental Research Advisory Committee (BERAC).

**The Opportunity**

With the $21^{st}$ Century dawns what many have called the "biological century"–an era when advances in biology, spurred by achievements in genomic research, including the sequencing of the human genome, will bring revolutionary and unconventional solutions to some of our most pressing and expensive challenges in health, energy, the environment, and national security.

We will understand how living organisms interact with and respond to their environments so well that we will be able to use biology to produce clean energy, remove excess carbon dioxide from the atmosphere, and help clean up the environment. Our understanding of global climate change and our ability to accurately predict climate over decades to centuries will enable us to develop science-based solutions to minimize the impacts of climate change and to better plan for our Nation's future energy needs. Understanding the biological effects of low doses of radiation will lead to the development of science-based health risk policy to better protect workers and citizens. Understanding the fate and transport of environmental contaminants will lead the way to discovering innovative approaches for cleaning up the environment. Both normal and abnormal health—from normal human development to cancer to brain function—can be understood and improved using radiotracers, advanced imaging instruments, and novel biomedical devices.

**The Challenges**

*Understanding and predicting climate* – Advanced climate models are needed to describe and predict the roles of oceans, the atmosphere, sea ice, and land masses on climate. So too, the role of clouds in controlling solar and terrestrial radiation onto and away from the Earth needs to be better understood since it is the largest uncertainty in climate prediction. Moreover, the impacts of excess carbon dioxide in the atmosphere from human sources, including energy use, on Earth's climate and ecosystems need to be determined and possible mitigation strategies developed.

*A cleaner environment* – Environmental sciences are undergoing a revolution, thanks in large part to the same molecular tools that have revolutionized biology in the last few decades—synchrotron radiation, advanced imaging and microscopy, and modern genomics. At the same time, the importance and roles of microbes in the environment are just beginning to be understood. How do microbes impact the geochemical cycles in the earth? How do they respond to perturbations, such as contamination? How do contaminants move through the subsurface? And how can we use nature's own biogeochemical 'tricks' to help us clean up contaminated sites in the DOE weapons complex and other places?

*Technology for a healthier Nation* – At the crossroads of the physical and biological sciences is the promise of remarkable technology for tomorrow's medicine. Developments in imaging technology have the potential to revolutionize all of medical imaging with increases in sensitivity, ease of use, and patient comfort. Technological wonders are on the horizon, like an artificial retina that will restore vision to the blind.

*A new biology* – Can we understand the workings of biological systems well enough so that we can use nature's own principles of design to solve energy and environmental challenges? Understanding nature's array of multi-protein molecular machines and complex microbial communities, each with exquisitely precise and efficient functions and controls, will enable us to use and even redesign these molecular machines or communities to address DOE and national needs.

**The Investment Plan**

All BER R&D investments are evaluated against the Administration's R&D Investment criteria that include research and user facility relevance, quality, and performance. BER will continue its investments in core technologies and fundamental science needed to address these daunting challenges. BER believes that the most important scientific advances in the 21st century will occur at the interfaces between scientific disciplines such as biology, physics, chemistry, engineering, and information science. BER investments at these interfaces will enable: (1) the development of a new research infrastructure for understanding the function and control of biological systems that can be used to solve critical problems in energy and the environment; (2) an improved ability to predict climate on global and regional scales; (3) development of strategies to remove excess carbon dioxide from the atmosphere; (4) new science-based strategies for the remediation, and long-term monitoring of the environment; and (5) the development of unique devices and technologies for the medical community that improve our Nation's health.

**How We Work**

BER uses a variety of mechanisms to conduct, coordinate, and fund biological and environmental research. BER is responsible for planning and prioritizing all aspects of supported research, for conducting ongoing assessments to ensure a comprehensive and balanced portfolio that addresses DOE and national science needs, and for coordinating its research programs with those of other federal agencies. BER regularly seeks advice on its research programs from the scientific community and from its diverse stakeholders. BER supports research at national laboratories, universities, research institutes, and private companies, and maintains a strong research infrastructure across the biological and environmental sciences most relevant to the BER program.

**Advisory and Consultative Activities**

To ensure that resources are allocated to the most scientifically relevant and promising research, BER actively seeks external input using a variety of advisory bodies. BER regularly compares its programs to the scientific priorities recommended by the BERAC and by the standing committees created by the Office of Science and Technology Policy (OSTP). BER staff and BERAC both interact with and receive feedback from other programs and advisory committees across the Department including Advanced Scientific Computing Research; Basic Energy Sciences; Environmental Management; Energy Efficiency and Renewable Energy; Nuclear Energy, Science and Technology; Fossil Energy; and the National Nuclear Security Administration. BER program coordination across federal agencies also benefits from international and interagency working groups such as those of the Interagency Genomics and Biotechnology working groups, the combined Climate Change Science Program and U.S. Global Change Research Program, and the National Institutes of Health Bioengineering Consortium. BER is currently having its Genomics: GTL program, including the GTL Roadmap, reviewed by the National Academies of Science. Finally, BER consults regularly with groups like JASON, involving physicists, mathematicians, engineers, etc., to receive feedback on BER program elements such as the Atmospheric Radiation Measurement (ARM) program, climate change prediction activities, the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), and the genomics program.

**Facility Operations Reviews**

All BER facility operations are monitored by peer reviews and user feedback. BER facility operations have also been reviewed by BERAC and by a 1999 OSTP interagency working group evaluating structural biology user facilities. In FY 2005, the Office of Science's Construction Management Support Division has reviewed BER's Environmental Molecular Sciences Laboratory. BER manages all facilities in a manner that meets user requirements as indicated by achieving performance specifications while protecting the safety of workers and the environment. Facilities are operated reliably and according to planned schedules. Facilities are also maintained and improved to remain at the cutting edge of technology and scientific capability.

**Program Reviews**

Effective program review, merit review, and user feedback are critical tools for BER to measure performance of research programs, research projects, and user facilities. The quality and scientific relevance of the BER program and its individual research projects are maintained by rigorous peer reviews conducted by internationally recognized scientific experts. The criteria for determining scientific quality and relevance include scientific merit, appropriateness of the proposed approach, and reasonableness of the requested level of funding, research facilities, and qualifications of the principal investigator. BER expects the highest quality research and, when necessary, takes corrective management actions based on results of the reviews. A measure of the quality of the BER research is the sustained achievement in advancing scientific knowledge. This is demonstrated by the publication of research results in the leading refereed scientific journals pertinent to BER-related research fields, by invited participation at national and international scientific conferences and workshops, and by honors received by BER-supported researchers.

At the highest level, regular reviews of individual BER program elements and of the entire BER research program are conducted by BERAC. As noted above, BER also benefits from interagency and international reviews of programs such as the Climate Change Science Program and the structural biology research program, including reviews by Boards and Committees of the National Academies of Science.

BER goes one step further in conducting program reviews. Panels of distinguished scientists are regularly charged with evaluating the quality of individual programs and with exploring ways of introducing new ideas and research performers from different scientific fields. This strategy is based on the conviction that the most important scientific advances of the new century will occur at the interfaces between scientific disciplines, such as biology and information science. The BER program is ideally positioned to facilitate and foster interactions between the physical sciences, the computational sciences, the environmental sciences, and the life sciences, and aggressively pursues every opportunity to nurture collaborations at the interfaces between these scientific domains.

**Planning and Priority Setting**

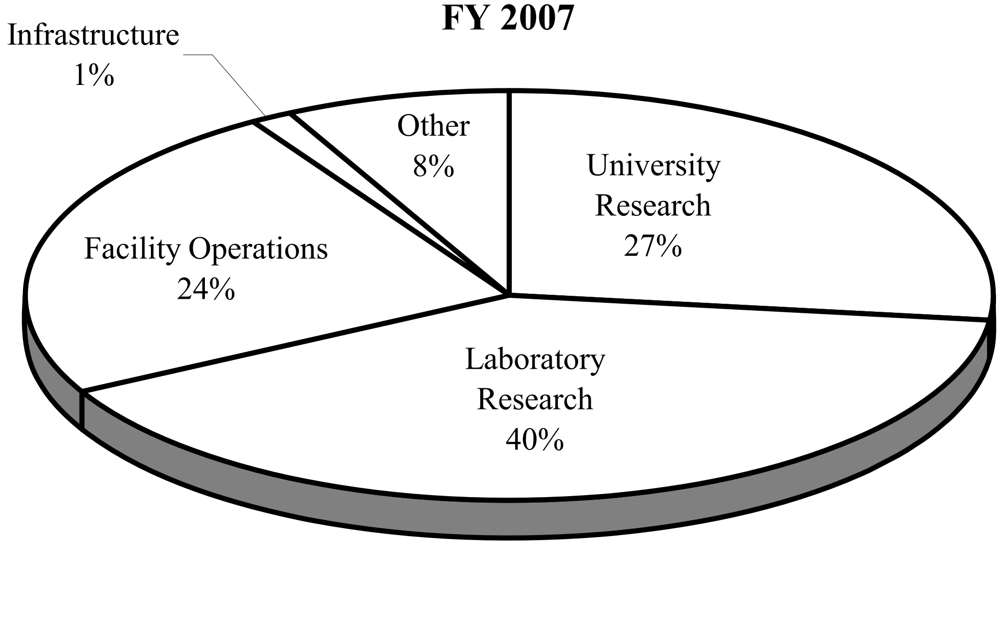
BER prides itself on supporting research and developing new research initiatives that lead the way across many fields of science and that effectively bring together many different disciplines, including biology, chemistry, engineering, computing, and the physical sciences. Merit reviews and user feedback are incorporated as BER anticipates and plans for the future needs of DOE research in the life and environmental sciences. This includes planning for future directions, opportunities, and initiatives within the BER research portfolio; maintaining the flexibility to quickly move into promising new areas; contributing to the health of the educational pipeline in critical subfields and disciplines; planning for upgrades at existing facilities to expand the research capabilities or operational capacity; ensuring the proper balance between facilities and research; and planning for future facilities necessary to advance the science in areas relevant to BER's mission with strong involvement of the research community.

BER planning and priority setting are also key BERAC activities and part of BER's interagency coordination. Individual BER program elements, e.g., human genome, low dose radiation research, Genomics: GTL, bioremediation research, global climate change, and medical applications develop long-range program plans through coordinated efforts with BERAC and other federal agencies.

**How We Spend Our Budget**

The BER budget has three major components: basic research at universities (27%); basic research at national laboratories (40%); and user facility support (24%). The remaining 9% includes general plant projects and equipment that supports the research infrastructure at the National Laboratories (1%) and all other research activities (primarily other federal agencies and industry (8%)). Research at national laboratories also includes Unmanned Aerial Vehicles and other elements that represent a research infrastructure for the scientific community that includes both university and laboratory scientists. BER's user facilities include the infrastructure at synchrotron and neutron sources for structural biology and the environmental sciences, operation and equipment for the Environmental Molecular Sciences Laboratory (EMSL), support for high-throughput DNA sequencing at the Joint Genome Institute, Atmospheric Radiation Measurement Infrastructure, Free-Air $CO_2$ Enrichment (FACE) experimental facilities, and for the Laboratory for Cooperative and Functional Genomics ("Mouse House").

**Biological and Environmental Research Budget Allocation FY 2007**



## Research

In FY 2007, the BER program will support fundamental research in climate change, environmental remediation, genomics, proteomics, radiation biology, and medical sciences at over 200 public and private research institutions in over 40 states, and at 14 DOE laboratories in 10 states. This research will be conducted in over 1,000 different research projects by over 2,500 researchers and students. In addition to the principal investigator for each research project funded by BER, individual projects typically have between 1 and 20 additional Ph.D.-level scientists who are funded collaborators. Information on scientific collaborators is not routinely tracked.

- ***University Research:*** University researchers play a critical role in the BER program, conducting fundamental research and developing the next generation of scientists for the nation's biological and environmental research efforts. BER will continue its commitment to and dependence on scientists at the Nation's universities. In general, BER-supported research at universities and research institutions are single investigator projects. Approximately half of BER basic research funding supports university-based activities directly and indirectly. University scientists are the major scientific users at BER facilities that include the ARM program, DNA sequencing, structural biology, FACE, EMSL, and the Laboratory for Comparative and Functional Genomics.

  All research projects supported by the BER program undergo regular merit review and evaluation based on the procedures set down in 10 CFR Part 605 for the extramural grant program (http://www.science.doe.gov/grants/merit.html). Peer review of BER projects is performed to provide an independent assessment of the scientific and/or technical merit of the research by peers having knowledge and expertise equal to that of the researchers whose work they review.

- ***National Laboratory Research:*** Research projects at national laboratories are most often multi-investigator team projects that take advantage of unique resources, capabilities, or facilities found at the national laboratories. Researchers at the national laboratories collaborate extensively with academic researchers supported by BER as well as with academic users of the BER facilities infrastructure including the EMSL, ARM, FACE, Environmental Remediation Sciences Research Field Research Center (FRC), the Joint Genome Institute (JGI), and the structural biology and environmental user facilities at the synchrotron.

  All DOE laboratory research projects supported by the BER program undergo regular merit review and evaluation. BER research at the DOE Laboratories and scientific user facilities undergoes peer review and evaluation in a similar procedure to that used for university-based research.

## BER Leadership and Unique Roles

The BER program has a broad range of unique roles for the Department and the national and international scientific communities including:

- Manage research on microbes for energy and the environment, and work with the Advanced Scientific Computing Research program to develop the computational methods and capabilities needed to advance understanding of complex biological systems, predict their behavior, and use that information to address DOE needs;
- Provide the research infrastructure needed to (1) characterize the multi-protein complexes that result in microbial products and processes of use to DOE, and (2) determine the functional repertoire of complex microbial communities that can be used to address DOE needs;
- Provide world-class structural biology user facilities;

- Provide cutting edge technologies, facilities (including high-throughput community DNA sequencing capabilities), and resources, including animal models, for genomics research;
- Provide world-class scientific user facilities for environmental and climate change research;
- Provide world leadership in low dose radiation research;
- Provide world leadership in the understanding of how metal and radionuclide contaminants interact with the environment and how environments respond to their presence;
- Provide world leadership in ground-based measurement of clouds and atmospheric properties to resolve key uncertainties in climate change, through the ARM program;
- Develop advanced predictive capabilities using coupled climate models on the Nation's premier computers for decade-to-century long simulations of climate change;
- Support fundamental research on carbon sequestration to develop technologies that enhance the uptake of carbon in terrestrial and ocean ecosystems;
- Provide the scientific knowledge and enabling discoveries to reduce the risks and costs associated with the cleanup of the DOE weapons complex and provide a basis for similar mission needs related to energy, water, and the disposal and storage of waste;
- Provide world leadership in support of science at the interface of physics, chemistry, materials, and computation to develop an artificial retina; and
- Ensure that the rights and welfare of human research subjects at the Department are protected while advances in biomedical, environmental, nuclear, and other research lead to discoveries that benefit humanity.

**Significant Program Shifts**

- BER will focus research activities on higher priorities, especially GTL, in support of Departmental goals and objectives. Funding reductions are initiated in the Environmental Remediation Research and in the Climate Change Research Subprograms. High level waste (including waste in storage tanks), ocean sciences, and carbon sequestration research are terminated within these two subprograms.

**Genomics: GTL Research**

The FY 2007 budget includes funds for the continued expansion of the Genomics: GTL program—a program at the forefront of the biological revolution. This program employs a systems approach to biology at the interface of the biological, physical, and computational sciences to address DOE's energy, environment, and national security mission needs. This research will continue to more fully characterize the inventory of multi-protein molecular machines found in selected DOE-relevant microbes and higher organisms. It will determine the diverse biochemical capabilities of microbes and microbial communities, especially as they relate to potential biological solutions to DOE needs, found in populations of microbes isolated from DOE-relevant sites. GTL research will provide the scientific community with knowledge, resources, and tools that benefit large numbers of research projects with positive impacts on more scientists and students than are negatively impacted by the initial reduction.

Development of a global biotechnology based energy infrastructure requires a science base that will enable scientists to redesign specific proteins, biochemical pathways, and even entire plants or microbes. Biofuels could be produced using plants, microbes, or isolated enzymes. Understanding the biological mechanisms involved in these energy producing processes will allow scientists and technologists to design novel biofuel production strategies involving both cellular and cell free systems that might include defined communities of microbes and engineered nanostructures. Within the Genomics: GTL program, BER will develop the understanding needed to advance biotechnology-based strategies for biofuel production, focusing on biohydrogen and bioethanol.

**Biological Production of Hydrogen**–Some microorganisms produce hydrogen naturally, and biotechnologies based on these microbial systems will lead to the development of clean, renewable sources of hydrogen. Under certain conditions, green algae and a type of bacteria known as cyanobacteria can use energy from the sun to split water and generate hydrogen. This process, known as biophotolysis, has the potential to produce hydrogen on the scale necessary for meeting future energy demand. This approach to hydrogen production is promising because it uses water as a source of hydrogen—a clean, renewable, carbon-free (i.e., non-fossil fuel based), substrate available in virtually inexhaustible quantities. Another advantage of biophotolysis, compared to engineered systems that capture and use sunlight, is the more efficient conversion of solar energy to hydrogen. Using and improving microbial systems to directly produce hydrogen from water eliminates inefficiencies associated with hydrogen production from biomass, such as producing and harvesting the biomass itself. Theoretically, the maximum energetic efficiency for direct biophotolysis is 40% compared with a maximum of about 1% for hydrogen production from biomass (Critical Reviews in Microbiology 31, 19-31, 2005). Fundamental research will be supported to understand biophotolysis, and other processes, well enough that predictive models of hydrogenase (the enzyme that cleaves water to produce hydrogen) structure and function, genetic regulatory and biochemical networks, and eventually entire microbes can be developed. Research will include investigations on a range of hydrogen-producing enzymes and organisms, understanding how hydrogenases work, the inhibition of hydrogenase activity by oxygen, and genetic regulatory and biochemical processes that influence hydrogen production. This new knowledge will be used to engineer the ideal microbe to use in hydrogen bioreactors or the ideal enzyme-catalyst to use in bioinspired nanostructures for hydrogen production.

**Cellulose to Ethanol–Advanced Biological Production of Ethanol**—Ethanol produced from corn starch is currently the most widely consumed biofuel in the United States, used as a substitute or octane booster for gasoline. A gallon of ethanol has about two-thirds the energy content of a gallon of gasoline. The production of cellulosic ethanol from biomass has promise for meeting a significantly larger portion of U.S. gasoline demand. A recent report ("Biomass as Feedstock for a Bioenergy and Bioproducts Industry:  The Technical Feasibility of a Billion-Ton Annual Supply," available from Oak Ridge National Laboratory, Oak Ridge, TN 37831; ORNL/TM-2005/66) has projected that relatively modest changes in the use of farmlands and forests could produce more than 1.3 billion dry tons of biomass per year, enough to reduce current oil demand by at least one-third given conservative estimates of conversion efficiencies. Research will be supported that provides a systems-level understanding of biological processes for developing and deploying large-scale, environmentally sound biotechnologies to produce ethanol from plant cell walls, primarily cellulose. Currently, a biochemical conversion of biomass to ethanol involves three basic steps: (1) breakdown of raw biomass using heat and chemicals, (2) use of enzymes to breakdown plant cell wall materials into simple sugars, and (3) conversion of the sugars into ethanol using microbes. The long-term goal is to integrate the bioprocessing into a single step. Accomplishing this requires the development of genetically modified, multifunctional microbes or a stable mixed culture of microbes capable of carrying out all biologically mediated transformations needed for the complete conversion of biomass to ethanol. Research will be supported on a variety of enzymes and microbes that contribute (individually and together) to the conversion of cellulose to ethanol; analysis of enzymes to understand how they interact with and breakdown cellulose; a determination of the factors, such as temperature and different combinations of sugars,  that influence biomass degradation or ethanol production; strategies for producing and maintaining stable mixed cultures of microbes; and improved capabilities for genetically engineering microbes that produce bioethanol. This research will lead to increased understanding of microbe-based production of cellulosic ethanol, increased production efficiencies, and reduced costs that will make cellulosic ethanol a cost-competitive alternative to gasoline in the coming decades.

**Climate Change Science Program**

In 2003, the Administration launched the Climate Change Research Initiative (CCRI) to focus research on areas where substantial progress in understanding and predicting climate change, including its causes and consequences, is possible over the next five years. The CCRI was then combined with the existing U.S. Global Change Research Program (USGCRP) to form a combined USGCRP/CCRI managed as the Climate Change Science Program (CCSP) by the cabinet-level Committee on Climate Change Science and Technology Integration. (The BER request for CCSP for FY 2007 is $126,187,000.) DOE, in conjunction with its interagency partners, including NSF, NASA, NOAA, USDA, Interior, and EPA, will continue to focus its Climate Change Research in CCSP priority areas. These areas include advanced climate modeling, critical climate processes (including effects of clouds and water vapor on the atmospheric radiation balance), carbon cycling, atmospheric composition (with a focus on both greenhouse gas concentrations and effects of various aerosols on climate), effects of climate change on important terrestrial ecosystems, and the development and evaluation of tools for assessing the economic costs and benefits of climate change and the different potential options for mitigation and adaptation to such change. The deliverables from this BER research will be highlighted by information useful to policy makers.

In FY 2007, BER will contribute to the CCRI from four programs: Terrestrial Carbon Processes, Climate Change Prediction, ARM, and Integrated Assessment. Activities will be focused on (1) helping to resolve the North American carbon sink question (i.e., the magnitude and location of the North American carbon sink); (2) deployment and operation of a mobile ARM Cloud and Radiation Testbed facility to provide data on the effects of clouds and aerosols on the atmospheric radiation budget in regions and locations of opportunity where data is lacking or sparse; (3) using advanced climate models to simulate potential effects of natural and human-induced climate forcing on global and regional climate and the potential effects on climate of alternative options for mitigating increases in human forcing of climate; and (4) developing and evaluating assessment tools needed to study costs and benefits of potential strategies for reducing net carbon dioxide emissions.

**Scientific Discovery through Advanced Computing (SciDAC)**

The Scientific Discovery through Advanced Computing (SciDAC) program is a set of coordinated investments across all Office of Science mission areas with the goal of achieving breakthrough scientific advances via computer simulation that are impossible using theoretical or laboratory studies alone. The power of computers and networks is increasing exponentially. Advances in high-end computing technology, together with innovative algorithms and software, are being exploited as intrinsic tools for scientific discovery. SciDAC has also pioneered an effective new model of multidisciplinary collaboration among discipline-specific scientists, computer scientists, computational scientists, and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can productively exploit terascale computing and networking resources. The program is bringing computation and simulation to parity with experiments and theory in the scientific research enterprise as demonstrated by major advances in climate modeling and prediction, plasma physics, particle physics, accelerator design, astrophysics, chemically reacting flows, and computational nanoscience.

In FY 2007, BER will continue to advance the science of climate modeling by coupling models of different components of the earth system related to climate and by significantly increasing the spatial resolution of global climate models. These SciDAC-enabled activities will allow climate scientists to gain unprecedented insights into potential effects of energy production and use on the global climate system.

BER will add a SciDAC component to GTL and Environmental Remediation research. GTL SciDAC will initiate new research to develop mathematical and computational tools needed for complex biological system modeling and for analysis of complex data sets, such as mass spectrometry data. Environmental Remediation SciDAC will provide an opportunity for subsurface and computational scientists to develop and improve methods of simulating subsurface reactive transport processes on "discovery class" computers. The intent is to explore potential advantages that high-end computing can bring to the understanding of optimal model complexity, the scalability of biogeochemical reactions, model abstraction methods, sources of uncertainty, parameter estimation and characterization measurements as input in subsurface reactive transport modeling.

**Scientific Facilities Utilization**

The BER request includes funds to maintain support of the Department's major scientific user facilities. BER has expanded the definition of a scientific user facility to include facilities such as structural biology research beam lines at the synchrotron light sources and neutron sources; the operation of the William R. Wiley Environmental Molecular Sciences Laboratory where research activities underpin long-term environmental remediation and other DOE missions in energy and national security; the Production Genomics Facility; the Laboratory for Comparative and Functional Genomics ("Mouse House"); and the ARM and FACE facilities. With this funding, BER will provide for the operation of the facilities, assuring access for scientists in universities, federal laboratories, and industry. BER will also leverage both federally and privately sponsored research to maintain support for and operation of these facilities.

BER will maintain and operate its user facilities so that the achieved operation time will be greater than 98%, on average, of total scheduled annual operation.

## User Statistics

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| | Actual | Estimated | |
| EMSL | | | |
| Optimal hours | 4,365 | 4,365 | 4,365 |
| Scheduled hours | 4,365 | 4,365 | 4,365 |
| Operation Time | 95% | 95% | >98% |
| Users[a] | 1400 | 1600 | 1700 |

[a] EMSL users are both onsite and remote. Individual users are counted once per proposal in a reporting period regardless of the number of visits or accesses but individual scientists could be counted as more than one user if they are part of independently merit reviewed proposals.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| | Actual | Estimated | |
| Production Genomics Facility (PGF) | | | |
| Optimal hours | 8,400 | 8,400 | 8,400 |
| Scheduled hours | 8,400 | 8,400 | 8,400 |
| Operation Time | >98% | >98% | >98% |
| Users[a] | 50 | 80 | 120 |
| Laboratory for Comparative and Functional Genomics ("Mouse House") | | | |
| Optimal hours | 3,536 | 3,536 | 3,536 |
| Scheduled hours | 3,536 | 3,536 | 3,536 |
| Operation Time | >99% | >99% | >99% |
| Users[b] | 20 | 20 | 20 |
| Atmospheric Radiation Measurement (ARM) | | | |
| Optimal hours | 7,884 | 7,884 | 7,884 |
| Scheduled hours | 7,884 | 7,884 | 7,884 |
| Operation Time | >98% | >98% | >98% |
| Users[c] | 800 | 800 | 850 |
| Free Air Carbon Dioxide Enrichment (FACE) | | | |
| Optimal hours | 3,865 | 3,865 | 3,865 |
| Scheduled hours | 3,865 | 3,865 | 3,865 |
| Operation Time[d] | >95% | >95% | >96% |
| Users | 150 | 150 | 195 |

User statistics for BER structural biology user facilities at DOE neutron and light sources are included as part of the user statistics collected and reported by the Basic Energy Sciences (BES) program and are not repeated here.

## Construction and Infrastructure

BER will meet the cost and schedule milestones for construction of facilities and major items of equipment within 10% of baseline estimates.

For BER activities the capital equipment is held approximately at near the FY 2006 level.

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[a] All users are remote. Primary users are individuals associated with approved projects being conducted at the PGF in a reporting period. Each user is counted once per year regardless of how many proposals their name may be associated with.

[b] Users are both remote and onsite. A user is defined as a research group with a project that uses the facility. Each group is counted only once regardless of how many visits or individual staff in the group use the facility.

[c] ARM users are both onsite and remote. A user is an individual who accesses or uses equipment or computers at an ARM site. Individuals are only counted once per reporting period at an individual site but may be counted at different ARM sites if they are a user at more than one site.

[d] FACE users are both onsite and remote. Individuals are counted once per proposal in a reporting period regardless of the number of visits or accesses but individual scientists could be counted as more than one user if they are part of independently merit reviewed proposals. An onsite user who uses more than one FACE site is counted once for each of the sites used to carry out the research unless the research is to compare results between multiple FACE sites.

The BER program, as part of its responsibilities as landlord for the Pacific Northwest National Laboratory (PNNL) and the Oak Ridge Institute for Science and Education (ORISE), provides funding for the general plant projects (GPP) and general purpose equipment (GPE). In addition to the general-purpose line item projects funded out of the Science Laboratories Infrastructure program, GPP and GPE represent the capital investment funding provided by the Department for the general laboratory infrastructure. This ensures that the PNNL and ORISE infrastructures will continue to enable the Department's mission activities at these sites.

**Workforce Development**

Workforce development is an integral and essential element of the BER mission to help ensure a science-trained workforce, including researchers, engineers, science educators, and technicians. The research programs and projects at the National Laboratories, universities, and research institutes actively integrate undergraduate and graduate students and post-doctoral investigators into their work. This "hands-on" approach is essential for the development of the next generation of scientists, engineers, and science educators. Specific fellowship programs are also sponsored by BER to target emerging areas of need in global change research. About 1,400 graduate students and post-doctoral investigators will be supported at universities and at National Laboratories in FY 2007, including those conducting research at BER user facilities with BER or other funds. BER will continue its support for graduate students and post-doctoral investigators in FY 2007.

Office of Science user facilities are playing an increasingly important role in workforce development. Graduate and postdoctoral students from many different disciplines use Office of Science user facilities. For example, researchers in the environmental, biological, and physical sciences use the instruments at EMSL and the synchrotron light sources. The unique capabilities at these facilities provide graduate and postdoctoral students the opportunity to participate in leading-edge research. Approximately half of all DOE facility users are graduate or postdoctoral fellows, for example some 600 to 700 students will conduct research at EMSL in FY 2007. Students who use EMSL receive their funding from a number of sources including the EMSL user (operating) budget, other BER projects, other DOE programs, other federal agencies, international sponsors, and private industry.

The fastest growing user community at the synchrotron light sources is environmental researchers. BER is working with BES, and BER provides funding to each of the synchrotron light sources for environmental researchers. This funding provides user support for BER sponsored scientists as well as maintenance and upgrade of environmental user stations. In addition, BER is working with scientists in the environmental research community who receive funding from DOE and other agencies to develop more environmental science user stations at the synchrotron light sources. This will further increase the impact of SC facilities on workforce development in important research fields, such as the environmental sciences.

BER will continue its commitment to and dependence on research scientists at the Nation's universities. Approximately half of BER basic research funding directly or indirectly supports university-based activities. University scientists are the major users at BER facilities and other enabling research infrastructure. University-based scientists are an integral part of research programs across the entire range of the BER portfolio. These scientists are funded through individual peer-reviewed grants and as members of peer-reviewed research teams involving both national laboratory and university scientists.

University-based scientists are the principal users of BER user facilities. University scientists also form the core of the science teams in the Climate Change Research Programs that network with the broader academic community as well as with scientists at DOE laboratories and other agencies, such as the

National Aeronautics and Space Administration and the National Oceanic and Atmospheric Administration. In addition, university-based scientists are funded through Requests for Applications across the entire BER program including genomics, structural biology, low dose radiation research, climate change research, bioremediation research, medical imaging, and radiopharmaceutical development. Furthermore, university scientists work in close partnership with scientists at National Laboratories in many other BER programs including genomics, and carbon sequestration research.

| | FY 2005 | FY 2006 est. | FY 2007 est. |
|---|---|---|---|
| # University Grants | 855 | 700 | 700 |
| Average Size per year | $300,000 | $250,000 | $250,000 |
| # Laboratory Projects | 400 | 375 | 350 |
| # Permanent Ph.D.s[a] (FTEs) | 1,540 | 1,321 | 1,291 |
| # Postdoctoral Associates[b] (FTEs) | 400 | 299 | 297 |
| # Graduate Students[k] (FTEs) | 500 | 436 | 423 |
| # Ph.D.s awarded[c] | 125 | 100 | 105 |

### External Independent Reviews

Beginning in FY 2005, the costs of conducting External Independent Reviews (EIRs) for Capital Asset Projects greater than $5,000,000 within SC have been funded by SC. Examples of EIRs include conducting Performance Baseline EIRs prior to Critical Decision-2 (CD-2) to verify the accuracy of cost and schedule baseline estimates and conducting Construction/Execution Readiness EIRs, which are done for all Major System projects prior to CD-3. These funds, which are managed by the Office of Engineering and Construction Management, are exclusively used for EIRs directly related to these projects funded within SC. Beginning in FY 2007, the EIR business line will be financed via the Working Capital Fund to achieve parity on how EIRs are funded and to standardize the administration of these critical activities.

[a] Estimated. Information is not readily available on the total number of permanent Ph.D. scientists associated with each research project. In addition to the principal investigator for each research project funded by BER, individual projects typically have between 1 and 20 additional Ph.D.-level scientists who are funded collaborators. Information on scientific collaborators is not routinely tracked.

[b] Estimated for national laboratory projects.

[c] Information is not available on the number of Ph.D.s awarded as a result of BER funded research at universities or national laboratories. Data is estimated.

## Life Sciences

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Life Sciences | | | |
| Structural Biology | 21,859 | 15,084 | 15,300 |
| Molecular and Cellular Biology | 103,669 | 109,670 | 159,942 |
| Human Genome | 62,941 | 62,885 | 74,575 |
| Health Effects | 10,174 | 8,808 | 7,321 |
| SBIR/STTR | — | 5,548 | 7,020 |
| Total, Life Sciences | 198,643 | 201,995 | 264,158 |

### Description

The mission of the Life Sciences subprogram is to foster fundamental research in the biological and life sciences that will provide new insights and advance knowledge to underpin the Department of Energy's mission needs. Biotechnology offers the promise of revolutionary solutions to energy and environmental challenges facing DOE and the Nation. Fundamental Life Sciences research will deliver a new knowledge base for cost effective cleanup of environmental contamination, design of new strategies for enhanced capture of atmospheric carbon dioxide, and increased bio-based sources of fuel or electricity. The program will also deliver new knowledge underpinning rigorous, cost-effective standards to protect the health of DOE cleanup workers and the public, and for science-based decisions on DOE site cleanup.

### Benefits

Fundamental research is supported in genomics and the health effects of low dose radiation. DNA sequencing is used to understand the genetic and environmental basis of normal and abnormal biological function, from genes that make some people more sensitive to the adverse effects of low doses of radiation to the biochemical capabilities of complex microbial communities that could be used to produce clean energy, clean up or stabilize wastes *in situ*, or sequester excess atmospheric carbon dioxide. Resources are developed and made widely available for determining protein structures at DOE synchrotron, for high-throughput genetic studies using mice, and for high-throughput genomic DNA sequencing. New capabilities are developed in the Genomics: GTL program for understanding the structure, function, and regulation of multi-protein complexes from DOE-relevant organisms and of complex, DOE-relevant microbial communities – information needed to develop biotechnological solutions for DOE needs.

### Supporting Information

BER Life Sciences supports research in the following areas:

- Biological effects of low doses of ionizing radiation. The program works closely with scientists, regulators, and the public to ensure that the research results are available to develop a better scientific basis for adequately protecting people from the adverse effects of ionizing radiation.
- Genomics: GTL research, developing, together with the Advanced Scientific Computing Research program, experimental and computational resources, tools, and technologies to understand the

complex behavior of biological systems – from single microbes to communities of multiple microbial species. This information can be used to develop innovative biotechnology solutions for energy production, waste cleanup, and carbon management.

- A high-throughput DNA sequencing user resource to meet DNA sequencing needs of the scientific community.
- Resources, tools, and technologies to understand the function of human genes identified as part of the International Human Genome Project using the mouse.

Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes. This subprogram was reviewed as part of a BERAC review of the entire BER program in FY 2001 and by a BERAC Committee of Visitors (COV) in FY 2005. The next scheduled review of the Life Sciences subprogram by a BERAC COV will likely be in FY 2009.

**FY 2005 Accomplishments**

- Getting a Sense of Community: For the first time, both genomic and proteomic approaches have been used on a naturally occurring microbial community from an acid mine drainage site to characterize the "community genome" as well as the "community proteome" and promising insights into potential biotechnology strategies for remediation of toxic materials.
- Microbial Genome Clearinghouse—You May Have Already Won: DOE's Joint Genome Institute has developed a new clearinghouse (http://img.jgi.doe.gov/v1.0/main.cgi) that will help researchers analyze the deluge of DNA data on microorganisms. The site currently stores nearly 300 draft or completed genome sequences from archaea, bacteria, and other microbes, along with tools for sifting through the data. Besides basic information about the gene, its protein, and its function, visitors can summon diagrams illustrating which biochemical pathways the gene influences. Browsing tools make it easy to pinpoint similar genes in different organisms and compare them side by side.
- Spotlighting Cellular Processes: The ability to insert fiber-optic probes into living cells to watch cellular processes unfold has been developed. Biological probes, such as antibody molecules, are mounted on the tip of small fibers and pushed through a cell's outer membrane. When the probe encounters its target it triggers a detectable fluorescence signal. This system has been used to detect DNA damage from chemical carcinogen exposure and, for the first time, has enabled scientists to witness the onset of apoptosis, or programmed cell death, in real time. This exciting technology will now be adapted to monitor reactive oxygen species produced in live cells in response to low doses of ionizing radiation.
- Fixing Radiation Damage—It's When, Not What: The extreme radiation resistance of the microbe *Deinococcus radiodurans* has been shown to not be due to unusual or extra genes that less resistant bacteria lack, but rather that is due to regulatory alterations that permit them to use their repair mechanisms much more efficiently. This discovery may lead to the identification of ways to increase the radiation resistance of cells prior to radiation exposures.
- A Hypothetically Speaking, It's in the Genes: New approach for identifying "hypothetical genes" has been developed that combines experimental and computational analyses. Integrative approaches such as this offer valuable strategies for undertaking the enormous challenge of characterizing the rapidly growing number of "hypothetical" proteins that are found in each newly sequenced genome.
- Microbes Exchange Information to Clean Up Our Act: The genome of a microbe that can be used to clean up pollution by chlorinated solvents – a major category of groundwater contaminants that are

often left as byproducts of dry cleaning or industrial production has been determined. The newly determined DNA sequence provided evidence that the soil bacterium may have developed the metabolic capability to consume chlorinated solvents fairly recently, possibly by acquiring genes from a neighboring microbe in order to survive the increased prevalence of the pollutants. This proposed lateral gene transfer is part of a rapidly growing body of evidence that will dramatically change our understanding of distant and recent microbial evolution.

- Big Science Successes: From Sea to Mining See!: The work of BER-funded scientists was identified as two of the top science stories of 2004. Research on the Sargasso Sea, resulted in the discovery of more than a million new genes that had never been seen before including the startling result that a gene whose product had previously been thought of as a light receptor may be used by many marine bacteria to process carbon. Environmental genomics research focuses on a small microbial community inside an abandoned mine where the pH is extremely acidic. This research spotlights the value and potential of environmental genomics using advanced genome sequencing technologies to study the genomes of entire communities, research made possible by pioneering DOE investments in the genomic sequencing complex community DNA samples.
- Bringing Science Ethics to your Living Room: The TV documentary "Bloodlines: Technology Hits Home," (http://www.pbs.org/bloodlines/) won the top broadcast award of the National Association of Science Writers (NASW), the top science journalism award in the U.S. The topic of Bloodlines is the ethical, legal, and societal challenges emerging from the Human Genome Project and some of the difficulties and dilemmas caused by the interaction of cutting edge science and the law. "Bloodlines" was originally funded by the Ethical, Legal, and Social Issues element of the BER Human Genome Program.
- Stretching a Visual Point with DNA: Optical mapping is a technology to directly image a "stretched-out" molecule of genomic DNA using the unique locations of restriction enzyme cut sites as orientation markers along the length of the DNA. This technique has now been used to directly compare single genomic DNA molecules from a series of different microbes to identify and annotate DNA alterations between bacterial strains represented by several species, including a microbe whose genome has not yet been sequenced. The results suggest that genomic rearrangements and chromosomal breakpoints of an unsequenced microbe can be readily identified and annotated against a previously sequenced strain using optical mapping. This will speed the analysis of microbial genomes by comparative genomics by using information from previously sequenced microbial species.
- Performance Art by Diatoms: Diatoms are simple single-celled algae, covered with elegant and often very beautiful casings sculpted from silica. They share biochemical features of both plants and animals and are related to the organisms that make up the well known White Cliffs of Dover in England. Scientists have taken a big step toward resolving the paradoxical nature of these odd microbes by sequencing the genome of the marine diatom *Thalassiosira pseudonana.* Analyses of these genes and the proteins they encode confirm that diatoms, in their evolutionary history, apparently acquired new genes by engulfing microbial neighbors including, possibly, genes that provided the diatom with all the machinery necessary for photosynthesis. Diatoms occupy vast swaths of ocean and fresh water, where they play a key role in the global carbon cycle. Diatom photosynthesis yields 19 billion tons of organic carbon, about 40% of the marine carbon produced each year, and thus represent one of nature's key defenses against global warming. Progress in analyzing the diatom genome is also shedding light on how a diatom constructs its intricately patterned glass shell, progress that could benefit both materials and climate change scientists.

- Some Archaea Eat Their Dessert First: Scientists describe the use of genome based analyses of methane-oxidizing *Archaea* (evolutionarily ancient microorganisms) from deep-sea sediments to study the biological mechanisms controlling anaerobic methane oxidation. One current model suggests that relatives of methane-producing *Archaea* developed the capacity to consume methane to produce cellular carbon and energy. The new results show that nearly all of the genes typically associated with methane production are present in one specific group of these methane-consuming organisms, but appear to be "run backwards" so that they consume rather than generate methane. Importantly, the sequencing of this microbe was completed without a requirement for individual growth and culturing of each organism in the sediments, a capability that is becoming increasingly valuable since most microbes are not readily culturable. These genome-based observations provide a foundation for metabolic modeling of methane oxidation in the absence of oxygen in the deep ocean. This will lead to a better understanding of the role these organisms play in the flux of greenhouse gases from ocean to atmosphere, information that may illuminate how oceanic microbes participate in global carbon cycling and climate processes.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Structural Biology** ................................................... | **21,859** | **15,084** | **15,300** |
| ▪ **Basic Research**................................................... | **6,559** | **—** | **—** |

Basic Structural Biology research is terminated to support Genomics: GTL research. Support for characterization, including imaging, of multiprotein complexes and of gene regulatory networks is transferred to Genomics: GTL.

| | | | |
|---|---|---|---|
| ▪ **Infrastructure Development** ............................ | **15,300** | **15,084** | **15,300** |

BER develops and supports access to beam lines and instrumentation at DOE's national user facilities for the Nation's structural biologists. BER coordinates, with the NIH and the NSF, the management of experimental stations at DOE synchrotrons (Advanced Photon Source [APS], Advanced Light Source [ALS], and Stanford Synchrotron Radiation Laboratory [SSRL]). User statistics for all BER structural biology user facilities are included in the BES facility user reports. BER continually assesses the quality of the instrumentation at its experimental stations and supports upgrades to install the most effective instrumentation for taking full advantage of the facility capabilities as they are improved by DOE.

| | | | |
|---|---|---|---|
| **Molecular and Cellular Biology**............................. | **103,669** | **109,670** | **159,942** |
| ▪ **Microbial Genomics** ....................................... | **8,276** | **—** | **—** |

Microbial genomics is consolidated within Genomics: GTL.

| | | | |
|---|---|---|---|
| ▪ **Carbon Sequestration Research** .................... | **5,581** | **7,106** | **7,127** |

Microbes and plants play substantial roles in the cycling of carbon through the environment. Carbon sequestration research seeks to understand how plants and microbes work together to sequester atmospheric carbon dioxide. The program continues to leverage the genomic DNA sequence of the

| | (dollars in thousands) | |
|---|---|---|
| FY 2005 | FY 2006 | FY 2007 |

poplar tree, completed in FY 2004, supporting research to understand the poplar genome and proteome related to carbon utilization. Research will also focus on microbes that live in the poplar rhizosphere (root zone) to understand the role these microbes play in the transfer of carbon between the roots and the soil. The program will emphasize organisms and pathways that serve to increase long-term carbon storage to identify strategies that would lead to increased carbon storage in the poplar rhizosphere and surrounding soil, such as manipulation of the soil chemical environment to promote specific microorganisms or metabolic pathways. This research leverages BER's more fundamental microbial systems biology research in Genomics: GTL and BER's terrestrial carbon cycle research to evaluate options for molecular-based terrestrial carbon sequestration.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **Genomics: GTL** ................................................ | **72,637** | **85,486** | **135,319** |

Genomics: GTL is a microbe-based program at the forefront of the biological revolution - a systems approach to biology at the interfaces of the biological, physical, and computational sciences. Genomics: GTL offers the possibility of biotechnology solutions that can give us abundant sources of clean energy, such as ethanol from cellulose or biohydrogen, yet control greenhouse gases such as carbon dioxide, a key factor in global climate change, and that can help us clean up contamination of the environment.

Genomics: GTL will require a mix of fundamental research and development of novel capabilities for new high-throughput biological research, e.g., for protein production, molecular imaging, small molecule production, and proteomics. Over the long-term, it will support a combination of fundamental research and technology development; development and use of facility infrastructure that will efficiently and cost effectively generate much needed data for the scientific community much like DNA sequencing was moved from the research laboratory to sequencing facilities in the human genome project; and demonstration projects developed in partnership with other DOE offices such as Energy Efficiency and Renewable Energy, Fossil Energy, and Environmental Management to "field test" potential biotechnology solutions for DOE energy and environmental needs. The program focuses on scientific challenges that can be uniquely addressed by DOE and its National Laboratories in partnership with scientists at universities and in the private sector and will focus on high-throughput genomic-scale activities (e.g., DNA sequencing, complex computational analysis, imaging, and genomic protein-expression experimentation and analysis) that are beyond the reach of individual investigators or even small teams.

The broad goals of this research are shared with other agencies, such as the National Institutes of Health, the National Science Foundation, the Department of Agriculture, the Environmental Protection Agency, and private sector companies and will require coordination exceeding that of the Human Genome Project.

In FY 2007, the program continues to support a mix of large multidisciplinary research teams and smaller individual investigator projects to:

- develop computational models and the necessary algorithmic and computational tools needed to describe the biochemical capabilities of microbial communities; to integrate diverse data types and data sets into single models; and that accurately describe and predict the behavior of genetic regulatory networks;
- develop high-throughput approaches for isolating and characterizing microbial molecular machines;
- develop new technologies and strategies for imaging individual proteins and molecular machines inside microbes;
- develop new technologies for producing large numbers of microbial proteins and molecular tags to identify those proteins;
- develop microbe-based strategies for production of celluosic ethanol and hydrogen; and
- determine the societal and legal implications of genomics research and technology.

In FY 2007, research will also continue the high-throughput DNA sequencing of microbes and microbial communities. This DNA sequence information will continue to serve as the core of biological information needed to understand the control and function of molecular machines and complex microbial communities.

Technology development research relevant to proposed GTL user facilities is increased in FY 2007 to address key challenges. Research will be increased to develop new methods that enable scientists to "see" individual molecular machines at work inside microbes. This capability will provide information that is needed to understand the functions, regulation, and interactions of molecular machines. Aspects of proteome analysis are now very efficient and being used for large numbers of analyses. Research will be increased to improve the efficiency of components of the proteome "pipeline," including aspects of initial sample preparation, analysis of protein modifications, and development of capabilities of high-throughput metabolite analysis. Research will also be increased to improve methods for long-term analysis of complex microbial communities in controlled environments. Only by understanding how microbes live and work together in the environment can we take advantage of their capabilities to address DOE mission needs.

SciDAC research is initiated to develop mathematical and computational tools needed for complex biological systems modeling and for analysis of complex data sets, such as those generated by mass spectrometry.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and merit-reviewed processes.

The request greatly accelerates fundamental Genomics: GTL research, including SciDAC research, so that Genomics: GTL research progress will be maximized and the program is able to optimize use of potential future facility infrastructure. GTL research accelerates, including a focus on microbe-based generation of hydrogen, production of ethanol from cellulose, sequestration of carbon dioxide, and bioremediation. The program would include multiple research paths to avoid roadblocks and to optimize systems design options and would be coordinated across DOE programs (both within and outside SC), across federal agencies (including the Department of Agriculture, National Science Foundation, National Institutes of Health), and across DOE laboratories, academia, industry, and nongovernmental organizations. Increased SciDAC research would develop mathematical and computational tools needed for complex biological system modeling, for analysis of complex data sets, such as mass spectrometry, and to develop predictive models of complex microbial communities.

Within the request, $40,000,000 is for GTL research which will contribute biotechnology solutions for two biofuels: hydrogen and ethanol. Studies have suggested that, by 2100 biotechnology-based energy use could equal all global fossil energy use today. Bioethanol is derived from plant cell walls (cellulosic ethanol) and biohydrogen is produced from water using energy from the sun (biophotolytic hydrogen). Cellulosic ethanol is a carbon-neutral fuel that can already be used within today's energy infrastructure. Microbes or microbial processes are used to produce ethanol from plant biomass such as corn plants left after a corn harvest or energy crops such as poplar trees, that are specifically raised as biomass for energy production. Hydrogen is the ultimate carbon-free energy carrier that can be converted efficiently to energy in fuel cells with water as the only chemical by-product. Microbes, the planet's dominant photosynthetic organisms, exist that can use solar energy to convert water to hydrogen and oxygen, i.e., biophotolysis.

New knowledge on biophotolysis and hydrogenases will be used to engineer the ideal microbe to use in hydrogen bioreactors or the ideal enzyme-catalyst to use in bioinspired nanostructures for hydrogen production. New knowledge on the enzymes and microbes that contribute (individually and together) to the conversion of cellulose to ethanol will be used to develop genetically modified, multifunctional microbes or a stable mixed culture of microbes capable of carrying out all biologically mediated transformations needed for the complete conversion of biomass to ethanol in a single step.

Fundamental research will be supported to understand biophotolysis, and other processes, well enough that predictive models of hydrogenase (the enzyme that cleaves water to produce hydrogen) structure and function, genetic regulatory and biochemical networks, and eventually entire microbes can be developed. Research will include investigations on a range of hydrogen-producing enzymes and organisms, understanding how hydrogenases work, the inhibition of hydrogenase activity by oxygen, and genetic regulatory and biochemical processes that influence hydrogen production.

Research will also be supported on a variety of enzymes and microbes that contribute (individually and together) to the conversion of cellulose to ethanol; analysis of enzymes to understand how they interact with and breakdown cellulose; a determination of the factors, such as temperature and different combinations of sugars,  that influence biomass degradation or ethanol production; strategies for producing and maintaining stable mixed cultures of microbes; and improved capabilities for genetically engineering microbes that produce bioethanol.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Low Dose Radiation Research** ......................... | **17,175** | **17,078** | **17,496** |

The goal of the Low Dose Radiation Research program is to support research that will help determine health risks from exposures to low levels of ionizing radiation, information critical to adequately and appropriately protect people and to make the most effective use of our national resources. Information developed in this program will provide a better scientific basis for making decisions with regard to remediating contaminated DOE sites and for determining acceptable levels of human health protection, both for cleanup workers and the public, in the most cost-effective manner. Some research in this program is jointly funded with NASA's Office of Biological and Physical Research.

Radiation studies have traditionally been carried out using isolated cells and the responses of those cells were extrapolated to tissues and organisms. We now know that cells within tissues respond very differently to radiation than do isolated cells. This difference is greatest for very low dose exposures, or for very low dose rates, because in these situations, most of the cells in a tissue would not be irradiated at all. After these low-level exposures, the few irradiated/potentially-damaged cells in the tissue are mostly surrounded and heavily outnumbered by unirradiated/undamaged cells.

We now know that tissues often "protect" themselves from abnormal cells—such as a cell damaged by radiation—and defective cells may be stimulated to undergo "altruistic suicide." Tissue function is the culmination of a multicellular network coordinated by soluble endocrine, autocrine, and paracrine signals, and linked through a scaffolding of extracellular matrix that dynamically maintains homeostasis by regulating tissue composition, function, and phenotype. Emerging data shows that for low dose exposures it is the networked, multicellular responses, rather than the damage *per se*, that dictate whether homeostasis is restored or if pathology ensues. High dose exposure may corrupt normal signaling and moderate chronic irradiation may persistently alter cellular phenotype compromising the surveillance of abnormal cells and allowing aberrant cells to accumulate and proliferate.

In FY 2007, the program has an increased emphasis on systems biology concepts to place radiation induced bystander effects, adaptive response, and genomic instability data into the context of irradiated system (i.e. tissues). Bystander effects result from cell-cell communication (extracellular signaling) and are a type of early multicellular programmed response that attempts to re-establish homeostasis and eliminate abnormal cells. Adaptive response and multi-generational radiation-induced genomic instability may result from persistent network perturbations following radiation exposures.

In FY 2007, the program is also emphasizing the use of genome-based technologies to learn how cells communicate with each other in tissues in response to radiation, what causes cells and tissue to undergo different biological responses to radiation at different times, and how some people may be more sensitive to radiation while others are relatively resistant.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and selected through competitive and merit-reviewed processes. University scientists, competing for funds in response to requests for applications, conduct a substantial fraction of the research in this subprogram.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Human Genome** | **62,941** | **62,885** | **74,575** |
| ▪ **Joint Genome Institute** | **51,500** | **51,500** | **62,055** |

The Joint Genome Institute's (JGI) high-throughput DNA sequencing factory, the Production Genomics Facility (PGF) is focused on helping to meet the growing demand for DNA sequencing in the broader scientific community. Sequencing capacity will be increased to at least 50 billion base pairs in FY 2007 to support the increasing demand and need of the DOE research programs and the scientific community. The JGI's Community Sequencing Program (CSP) devotes 60% of its sequencing capacity to the merit-reviewed sequencing needs of the broader scientific community, including the needs of other agencies. DNA sequencing targets are chosen using peer review of requests for sequencing submitted by individual scientists and other federal agencies that share some DOE missions (for example USDA for Biomass). In FY 2007, the CSP will sequence approximately 30 billion base pairs of DNA from individual microbes, microbial communities, small plants and animals, and large plants and animals that will be selected by the CSP's merit review panel in FY 2006. Any large genomes selected for sequencing through the CSP will be required to meet the additional criteria of general relevance to DOE mission needs. Forty percent of the JGI's DNA sequencing capacity is being used to address DOE sequencing needs, including BER programs such as carbon sequestration research and bioremediation research, low dose radiation research and other DOE and national needs. The substantial high-throughput DNA sequencing needs of the GTL program ($10M) are supported at the JGI directly by the Genomics: GTL program and are not included here. These GTL funds support DNA sequencing and DNA sequencing research that present unique sequencing challenges primarily attributable to the complexity or difficulty of the environments from which the microbes or plants were isolated.

The JGI is a virtual research institute principally comprised of research programs at DOE national laboratories (LLNL, LANL, LBNL, PNNL, and ORNL). The JGI's DNA sequencing factory is located in Walnut Creek, California.

In FY 2007, the increased funding supports an increase of 15% in the DNA sequencing capacity for DOE and the scientific community.

| | | | |
|---|---|---|---|
| ▪ **Tools for DNA Sequencing and Sequence Analysis** | **9,594** | **9,785** | **10,520** |

BER continues to develop the tools and resources needed by the scientific, medical, and industrial sector communities to fully exploit the information contained in complete DNA sequences, including the first human genome sequence. Use of sequence information to understand human biology and disease will also require new strategies and tools capable of high-throughput, genome-wide experimental and analytic approaches. BER will continue efforts to develop high-throughput approaches for analyzing gene regulation and function.

The research activities in this subprogram are carried out at the JGI, national laboratories, universities, and private institutions and selected through competitive and peer-reviewed processes.

In FY 2007 the increased funding will support additional efforts to develop high-throughput annotation methods that keep pace with the rapidly increasing rate of DNA sequencing.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| | (dollars in thousands) | | |
| ▪ **Ethical, Legal, and Societal Issues (ELSI)** | **1,847** | **1,600** | **2,000** |

In FY 2007, ELSI research will increase and complete the refocusing of ELSI research on activities applicable to Office of Science issues in biotechnology and nanotechnology such as environmental or human health concerns associated with Genomics: GTL or nanotechnology research. Research with these funds will be coordinated across the Office of Science. The increased funding will support the first full year of research in the newly refocused ELSI program.

| | | | |
|---|---|---|---|
| **Health Effects** | **10,174** | **8,808** | **7,321** |

Functional genomics research is a key link between human genomic sequencing, that provides a complete parts list for a genome, and the development of information (a high-tech owner's manual) that is useful, in the case of human, in understanding normal human development and disease processes. The mouse continues to be the focus of our efforts. Research at BER's Center for Comparative and Functional Genomics user facility at Oak Ridge National Laboratory serves as a national focal point for high-throughput genetic studies using mice. This facility creates and genetically characterizes new mutant strains of mice that serve as important models of human genetic diseases and for understanding gene function especially as they relate to the genetic information found on human chromosomes 5, 16, and 19 (DOE's chromosomes in the International Human Genome Project). It also develops high-throughput tools and strategies to characterize these mice. This user facility provides tools useful to the entire scientific community for decoding the functionality of the human genome.

The research activities in this subprogram are principally carried out at National Laboratories, selected through merit-reviewed processes.

In FY 2007, the decreased funding will reduce research on animal models for disease associated with exposures to energy-related materials.

| | | | |
|---|---|---|---|
| **SBIR/STTR** | **—** | **5,548** | **7,020** |

In FY 2005 $4,816,000 and $577,000 were transferred to the SBIR and STTR programs, respectively. FY 2006 and FY 2007 amounts are the estimated requirements for continuation of the programs.

| | | | |
|---|---|---|---|
| **Total, Life Sciences** | **198,643** | **201,995** | **264,158** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Structural Biology** | |
| ▪ Structural Biology Infrastructure Development is held near FY 2006 levels. | +216 |
| **Molecular and Cellular Biology** | |
| ▪ Carbon Sequestration Research is held near FY 2006 levels. | +21 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ Genomics: GTL research will be increased to speed development of technologies that underpin proposed facility infrastructure including high-throughput methods for real time imaging of molecular machines inside microbial cells, for reducing current bottlenecks in high-throughput proteomics, and for improved methods for studying complex microbial communities in controlled environments. The increase also funds the following: greatly accelerates fundamental Genomics: GTL research, so that Genomics: GTL research progress will be maximized and the program is able to optimize use of potential future facility infrastructure. It also includes enhanced SciDAC Research, microbe-based generation of hydrogen and production of ethanol from cellulose, sequestration of carbon dioxide, and bioremediation. The program would include multiple research paths to avoid roadblocks and to optimize systems design options and would be coordinated across DOE programs (both within and outside SC), across federal agencies (including the Department of Agriculture, National Science Foundation, National Institutes of Health), and across DOE laboratories, academia, industry, and nongovernmental organizations. Increased SciDAC research would develop mathematical and computational tools needed for complex biological system modeling, for analysis of complex data sets, such as mass spectrometry, and to develop predictive models of complex microbial communities..... | +49,833 |
| ▪ Low Dose Radiation Research is held near FY 2006 levels. | +418 |
| **Total, Molecular and Cellular Biology** | **+50,272** |
| **Human Genome** | |
| ▪ Joint Genome Institute increases DNA sequencing capacity for DOE and the scientific community by an additional 15% to support increased scientific need for genomic DNA sequencing in BER programs and in the broader scientific community. Tools for DNA Sequencing and Sequence Analysis research increases to continue development of high-throughput approaches for analyzing gene regulation and function | +10,555 |
| ▪ Tools for DNA Sequencing and Sequence Analysis research increases to continue development of high-throughput approaches for analyzing gene regulation and function. | +735 |
| ▪ ELSI research increases to identify and understand the environmental or human health concerns of Genomics: GTL research… | +400 |
| **Total Human Genome** | **+11,690** |
| **Health Effects** | |
| ▪ Health Effects research decreases research on animal models for disease associated with exposures to energy-related materials. The support for the mouse user facility, the Center for Comparative and Functional Genomics, continues at FY 2006 levels. | -1,487 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **SBIR/STTR** | |
| ▪ Increases in SBIR/STTR due to increases in Life Sciences research funding. | +1,472 |
| **Total Funding Change, Life Sciences** | **+62,163** |

# Climate Change Research

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Climate Change Research | | | |
| Climate Forcing | 74,346 | 78,980 | 77,831 |
| Climate Change Modeling | 27,507 | 26,680 | 25,175 |
| Climate Change Response | 25,132 | 24,986 | 23,181 |
| Climate Change Mitigation | 8,550 | 6,947 | 5,014 |
| SBIR/STTR | — | 3,936 | 3,708 |
| Total, Climate Change Research | 135,535 | 141,529 | 134,909 |

### Description

The mission of the Climate Change Research subprogram is to deliver relevant scientific knowledge that will enable scientifically based predictions and assessments of the potential effects of greenhouse gas and aerosol emissions on climate and the environment.

### Benefits

This subprogram's research will reduce and resolve key uncertainties and provide the scientific foundation needed to predict, assess, and help mitigate adverse effects of energy production and use on the environment. This will be done through research on climate forcing and processes, including factors that affect climate forcing, such as clouds and aerosols and carbon cycling, climate change modeling and simulation to develop models needed to project what the likely response of the climate system would be in the future to natural and human-induced climate forcing, the response of ecological and human systems to ongoing and projected future changes in climate and atmospheric composition associated with energy production, and climate change mitigation, specifically research that could lead to the development of strategies or technologies for modifying or managing natural carbon sequestration processes in terrestrial systems to enhance their potential.

### Supporting Information

The Climate Change Research subprogram supports four contributing areas of research: Climate Forcing, including processes that affect climate forcing; Climate Change Modeling; Climate Change Responses; and Climate Change Mitigation. The research is focused on understanding the physical, chemical, and biological processes affecting the Earth's atmosphere, land, and oceans and how these processes may be affected, either directly or indirectly by changes in radiative forcing of climate resulting from energy production and use, primarily the emission of carbon dioxide from fossil fuel combustion, how the climate system would likely respond to human-induced and natural changes in radiative forcing, what the potential response would be of ecological and ecosystem systems to climatic changes, and how natural processes in terrestrial and ocean systems can be altered or managed to enhance their long-term capacity to sequester carbon dioxide emitted to the atmosphere, thereby helping to mitigate the increase in atmospheric $CO_2$. BER has designed and planned the research program to provide data that will enable objective assessments of the potential for, and consequences of, global warming. It is intended to provide a scientific basis that will enable decision makers to determine a "safe level" of greenhouse gases in the Earth's atmosphere to avoid a disruptive, human-induced interference in the climate system.

U.S. Climate Change Research is currently organized into the Climate Change Science Program (CCSP) and the Climate Change Technology Program (CCTP). The CCSP includes the interagency U.S. Global Change Research Program (USGCRP), proposed by the first President Bush in 1989 and codified by Congress in the Global Change Research Act of 1990 (P.L. 101-606), and the current Administration's Climate Change Research Initiative (CCRI).

The BER Climate Change Research subprogram (excluding the Climate Change Mitigation element which focuses on carbon sequestration in the terrestrial biosphere) represents DOE's contribution to the CCSP (USGCRP and CCRI). The Climate Change Mitigation/carbon sequestration element in Climate Change Research plus carbon sequestration activity in the Life Sciences subprogram are BER's contribution to the CCTP.

The CCRI is a set of cross-agency programs in areas of high priority climate change research where substantial progress is anticipated over the next three to five years. The specific focus areas include climate forcing (atmospheric concentrations of greenhouse gases and aerosols); climate feedbacks and sensitivity; climate modeling, including enabling research; regional impacts of climate change, including environment-society interactions; and climate observations. In FY 2007, BER will continue to participate in one of the specific research areas: climate forcing, which includes modeling carbon sources and sinks, especially those in North America. In FY 2007, BER will continue to support research to quantify the magnitude and location of the North American carbon sink, a high priority need identified in the interagency Carbon Cycle Science Plan, and on climate modeling, Atmospheric Radiation Measurement (ARM), and Integrated Assessment activities (BER's FY 2007 CCRI request is $23,750,000).

A major emphasis of the Climate Change Research subprogram is on understanding climate forcing, especially the radiation balance from the surface of the Earth to the top of the atmosphere and how changes in this balance due to increases in the concentration of greenhouse gases in the atmosphere may alter climate. Much of the research is focused on improving the quantitative models necessary to predict possible climate change at global and regional scales. Research in the ARM program will continue to focus on resolving the greatest scientific uncertainty in climate change prediction – the role of clouds and their interactions with solar radiation. ARM seeks to develop a better quantitative understanding of how atmospheric properties, including the extent and type of cloud cover and changes in aerosols and greenhouse gas concentrations, affect the solar and infrared radiation balance that drives the climate system. It also includes support to archive and analyze climate change data, including data from the ARM sites, and data on greenhouse gas emissions and concentrations and to make such data available for use by the broader climate change research community.

The Atmospheric Science program was reconfigured in FY 2005 to focus on acquiring the data needed to understand the atmospheric processes that control the transport, transformation, and fate of energy-related aerosols emitted to the atmosphere and their radiative properties so as to enable more reliable and accurate simulations of their radiative forcing effect on climate. In FY 2007, the program will continue studies of the physical, chemical, and radiative properties of aerosols and how much they may directly or indirectly affect the radiation balance.

Research on the carbon cycle explores the movement of carbon on a continental scale, starting from natural and anthropogenic emissions to ultimate sinks in the terrestrial biosphere and the oceans.

Experimental and modeling efforts primarily address the net exchange of carbon between major types of terrestrial ecosystems and the atmosphere. The focus in developing an understanding and ability to model the processes controlling the exchange of carbon dioxide between terrestrial systems and the atmosphere and how these processes may affect the atmospheric concentration of carbon dioxide which contributes to climate forcing.

Climate change modeling program element develops advanced, fully coupled, atmosphere-ocean-sea ice-land surface climate models and uses premier supercomputers to simulate and predict climate and climate change, including evaluating uncertainties in climate models due to changes in atmospheric levels of greenhouse gases on decade-to-century time scales. The focus is on developing, testing, improving, and applying state-of-the art climate models for assessing the potential for future climate changes due to natural and human-induced forcing of the climate system.

Ecological Processes research is focused on experimental and modeling studies to understand and predict the effects of climate and atmospheric changes on the biological structure and functioning of terrestrial ecosystems. The research also seeks to identify the potential feedbacks from ecosystems to climate and atmospheric composition. The research emphasizes major field studies of intact ecosystems using experimental manipulations of, for example, carbon dioxide and ozone concentrations and precipitation, and using data from these experiments to develop, test, and improve models for simulating and predicting ecosystem responses to environmental changes associated with energy production and use. The research also focuses on the causal mechanisms and pathways of biological and ecological responses ranging from the proteome of individual species to the whole ecosystem and will develop advanced computational models to establish how changes in the proteomes of single species or whole systems can explain the responses and behavior of complex ecosystems.

Human Interactions research is focused on improving methods and models that can be used to assess the economic and societal costs and benefits of both human-induced climate change and possible response options or strategies for mitigating or adapting to climate change.

The carbon sequestration element under Climate Change Mitigation funds basic research that seeks to exploit the biosphere's natural processes to enhance the sequestration of atmospheric carbon dioxide in terrestrial ecosystems. It also seeks the understanding needed to assess the potential environmental implications of purposeful enhancement and/or disposal of carbon in the terrestrial biosphere. The carbon sequestration activities include research to identify and understand the environmental and biological factors or processes that limit carbon sequestration in terrestrial systems and to develop approaches for overcoming such limitations to enhance sequestration. The research includes studies on the role of terrestrial microorganisms and terrestrial higher plants in carbon sequestration.

Periodic retrospective analysis is employed to evaluate program management processes, priorities, and outcomes. A BERAC COV for the Climate Change Research Program was established in FY 2004 to provide outside expert validation of the program's merit-based review and funding decision processes that impact scientific quality, programmatic relevance, and performance. The COV found the Climate Change Research subprogram to be a credit to DOE and an example of the way that Executive agencies should operate. It also found many of the programs within the subprogram to be unique. The COV concluded that the Climate Change Research programs are productive and support high quality research that plays an important role in the DOE and especially in the interagency U.S. Climate Change Science Program. The COV found the Climate Change Research subprogram to be generally well managed, but noted the need to improve documentation of the basis for proposal funding decisions, and the performance and outcomes of Climate Change Research programs. BER has taken action to address these findings.

The full report and the BER response are at http://www.science.doe.gov/ober/berac.html.

**FY 2005 Accomplishments**

- Release of New Version of Fully-Coupled Climate System Model: The most recent version of the Community Climate Model System, CCSM3.0, which is a fully coupled atmosphere-ocean-sea ice-land surface model, was released. Its release marks a significant milestone in the development of climate models that now incorporate the ability to simulate phenomena ranging from the effect of volcanic eruptions on temperature patterns to the impact of shifting sea ice on sunlight absorbed by the oceans. The model was developed at the National Center for Atmospheric Research in collaboration with researchers at universities and DOE laboratories, with major investments from DOE's climate modeling program. Model results and the underlying computer codes have been released to atmospheric researchers and other users worldwide. Scientists have applied the new model to generate scenarios of future potential climate change for use in preparing the Intergovernmental Panel on Climate Change's Fourth Assessment Report (IPCC AR4). Preliminary results of simulations of future climate states using CCSM3.0 indicate global temperatures could rise by 2.6 degrees Celsius (4.7 degrees Fahrenheit) in a hypothetical scenario in which atmospheric levels of carbon dioxide are suddenly doubled. That is significantly more than the 2 degree Celsius (3.6 degree Fahrenheit) increase that had been indicated by the preceding version of the model. In addition to simulating temperatures over the next century, scientists are using the model to study climate patterns of the past, such as the peak of the last ice age 21,000 years ago. It will also be used to probe chemical processes and the cycling of carbon between the atmosphere, ocean, and land, as well as the localized impacts of sulfates and other pollutants on climate.
- Climate Model Simulates Occurrence of Extreme Heat Wave Events Under Greenhouse Gas Forcing Climate Change Scenario: Results under a 'business-as-usual' scenario of future carbon dioxide emissions using a global coupled climate model indicate a distinct geographic pattern to future simulated changes in heat waves. Model results for areas of Europe and North America, associated with the severe heat waves in Chicago in 1995 and Paris in 2003, show that future heat waves in these areas will become more intense, more frequent, and longer lasting in the second half of the 21st century. Observations and the model results show that present-day heat waves over Europe and North America coincide with a specific atmospheric circulation pattern that is intensified by ongoing increases in greenhouse gases, indicating that it will produce more severe heat waves in those regions in the future. This research was jointly sponsored by BER and the National Center for Atmospheric Research.
- Regional Climate Model Simulates Global "Warming Hole" in Central United States: A local minimum warming ("warming hole") in summer over the central United States was predicted for the next few decades using a regional climate change model. Although the simulated daily maximum temperature in the "hole" increased in summer between the 1990s and 2040s, the simulated increase in the "hole" was 2.0-2.5°C (about 4°F) less than in the surrounding area. This projected "warming hole" coincides roughly with an observed "hole" in the warming of the last 25 years of the 20th century in the central United States. The simulation showed that the "hole" was associated with changes in low-level circulations that lead to replenishment of seasonally depleted soil moisture, thereby increasing late-summer evapotranspiration and suppressing daytime heating. These regional-scale feedback processes, which are unresolvable by most global climate models, may partly explain

the cooling trend in the central and eastern United States occurring in spite of global warming, and potentially could reduce the magnitude of future warming in the region due to the enhanced greenhouse effect caused by increasing carbon dioxide concentration in the atmosphere.

- ARM Mobile Facility (AMF) Completed and Deployed to Study Clouds and Aerosols: With instrumentation and data systems similar to ARM stationary sites at the North Slope of Alaska and the Tropical Western Pacific, fabrication of the AMF has been completed for deployment to sites around the world in various climatic regimes for durations of 6 to 18 months. Following a competitive peer review deployments were selected for 2005 and 2006. In 2005, researchers from the ARM Program deployed the facility at Pt. Reyes, California and in collaboration with scientists from the U.S. Office of Naval Research, NOAA, and DOE's Atmospheric Science Program began a 6-month campaign to study the interactions between marine stratus clouds and aerosols and the effect of such interactions on the absorption and scattering in incoming solar radiation and drizzle. The experiment addresses the specific effects of aerosols on the discrepancy between the measured and modeled amount of solar radiation absorbed by these clouds. In 2006, the AMF will be deployed at Niamey, Niger, Africa, as part of the field phase of the international African Monsoon Multidisciplinary Analysis (AMMA). The campaign will study meteorological conditions ranging from deep, tropical convective clouds in the humid tropical air masses prevalent in the wet season to the aerosol-laden dry air masses found during the dry season. These campaigns will provide unique opportunities for evaluating and improving the parameterization schemes used in climate models across a wide range of meteorological conditions.
- New Parameterization Improves Climate Simulations: The addition of a new ARM-developed parameterization scheme for convection to the Community Atmosphere Model (known as CAM3) has resulted in a remarkable improvement in the simulation of climate and its variability on intraseasonal timescales in the Tropics. In particular, several long-standing model biases, including the dual Intertropical Convergence Zones in the Equatorial Pacific Ocean are eliminated when the new parameterization is used in the model. The new parameterization improved simulations for precipitation in both winter and boreal summer seasons and more accurately simulates the annual cycle of the monsoon precipitation. The new convection parameterization also improves the simulation of tropical intraseasonal variability.
- Carbon Balance of Western Montane Coniferous Forest found to be Sensitive to Timing of Spring Warming: Montane forests are responsible for much of the atmospheric $CO_2$ assimilated by terrestrial ecosystems in the western United States. This poses challenges for accurate quantification of ecosystem carbon balance and dynamics because the current generation of $CO_2$ exchange measurement systems and approaches are designed to function in relatively flat, simple terrain. Using a specially designed multiple tower system, it was shown that when current measurement methods are deployed in mountainous terrain without special accommodation for the complex topography, the annual net $CO_2$ uptake by forests is underestimated by about 17%. When corrected for complex topography, a subalpine forest in Colorado was found to store about 100 g C $m^{-2}$ each year (5-year average). This annual net $CO_2$ uptake was sensitive to interannual climatic variation, with the most sensitive period being the early spring (April and May), when as much as 40% of the annual net $CO_2$ uptake can occur within a 30-day period. During years when spring warming occurred early, as is predicted for the future by climate models, annual net $CO_2$ uptake by the forest declined; this is contrary to studies in eastern deciduous forest ecosystems, where earlier spring warming is predicted to enhance annual net $CO_2$ uptake. This divergence may be due to differences

between the evergreen trees that dominate western forests and the winter-deciduous trees that dominate eastern forests.

- Genetic Diversity and Gene Expression of Carbon Fixation Influence Carbon Fixation and Potentially Carbon Sequestration in Gulf of Mexico area affected by Mississippi River Plume: The Mississippi River Plume strongly influences the biology, chemistry, physics, and the air-sea interactions of much of the Gulf of Mexico, including the atmospheric humidity and $CO_2$ levels of the southeastern United States. The biological processes occurring in this plume largely dictate whether it takes up or releases atmospheric $CO_2$. Using primary productivity and remote sensing analyses, it was shown that the offshore Mississippi River Plume is responsible for about 40% of the surface primary productivity in the low nutrient waters of the Gulf of Mexico. Nutrient uptake, biological productivity, and gene expression analyses revealed two alternative routes for $CO_2$ fixation in the Plume: (1) a cyanobacterial-driven uptake which likely leads to only short-term carbon storage in the ocean and (2) a diverse, diatom driven uptake which may contribute to longer-term carbon storage (removal from the atmosphere) in the ocean. The genetic sequence information that was collected will enable quantification of phytoplankton group-specific gene expression in the environment, providing new insights about the role of the Mississippi River Plume in controlling atmospheric $CO_2$ increase.

- Can Iron Fertilization of the Ocean be both Effective and Efficient at Sequestering Carbon? An investigation into the effectiveness of iron fertilization of the ocean surface as a means to increase the efficiency of the biological pump of carbon in waters of the Ross Sea, Antarctica was conducted using the CIAO ecosystem model. Results indicate that the stimulation of air-sea $CO_2$ exchange caused by iron fertilization depends primarily on the timing of the fertilization, regardless of the amount of iron added. Increasing the area of fertilization produced the largest response and increasing initial iron concentration produced the smallest, in the model. In all cases, as the intensity of iron fertilization increased, the fertilization efficiency ($CO_2$ uptake per unit iron added) dropped. Strategies that maximized the fertilization efficiency resulted in relatively little additional $CO_2$ being drawn out of the atmosphere. Conversely, to markedly increase oceanic uptake of atmospheric $CO_2$ would require the addition of large amounts of iron due to the low fertilization efficiencies associated with maximum air-sea $CO_2$ exchange.

- Hydrate Reactor Developed to Improve Efficiency of Deep Ocean Injection for Carbon Sequestration: A continuous-jet hydrate reactor was developed to efficiently produce dense, negatively buoyant (i.e., sinking) $CO_2$ hydrate particles for the purpose of carbon sequestration via direct injection of $CO_2$ into the deep ocean. The technical feasibility of the reactor was proven at Oak Ridge National Laboratory using a 72-liter seafloor process simulator and at the National Energy and Technology Laboratory using a high-pressure water tunnel facility. Field verification of laboratory results was demonstrated in Monterey Bay, California, using the facilities of Monterey Bay Aquarium Research Institute. Prior to this, methods for direct injection of $CO_2$ into the deep ocean were inefficient because the injection of liquid $CO_2$ alone produces buoyant droplets with the risk of returning to the ocean surface and atmosphere rather than remaining in the ocean for long periods required for effective carbon sequestration.

- Deep Ocean Injection of $CO_2$ harmful to deep-sea organisms: Effects of injected $CO_2$ on foraminiferal assemblages living at 3600 meter depth on the deep-sea floor were evaluated during the first field experiment off the coast of California. Foraminifera, commonly referred to as "forams" are single-celled protists with shells and range in size from 100 micrometers to almost 20 centimeters (cm). Most of the estimated 4,000 living species of forams are found in the world's oceans. Injection of $CO_2$ into the deep ocean has been proposed as means to sequester carbon and slow the increase in atmospheric $CO_2$ concentration. Results from this study imply almost complete initial mortality of forams and severe carbonate dissolution of the shells of forams in ocean sediments to depths of at least 10 cm into the sediment in close association to the point of $CO_2$ injection. This results in major decreases in the abundance and taxonomic diversity in both living and dead assemblages of forams on the sea floor. A second, shallower (3100 meter depth) experiment confirmed total mortality in at least the upper 1 cm of sediments and dissolution effects to even greater depths, which are still being determined. Benthic foraminifera are therefore now known to be highly vulnerable to $CO_2$ injection into the deep ocean.

- Forest Food Chain Dynamics Altered by Elevated Atmospheric Carbon Dioxide and Ozone Concentrations: BER constructed, maintains, and operates a large-scale field research facility in northern Wisconsin to study effects of experimentally elevated concentrations of carbon dioxide and ozone on the structure and functioning of hardwood forest ecosystems (concentrations of both gases are increasing because of energy production from fossil fuels). The forest being studied, a constructed mixture of aspen, birch, and maple trees, has been exposed to elevated carbon dioxide and ozone since 1997. Scientists recently discovered that elevated levels of these two gases can alter the feeding and reproduction of herbivorous insects, as well as their pheromone-mediated predator escape behaviors. For example, the efficacy of insect escape responses appears to increase under elevated $O_3$ but decrease under elevated $CO_2$. These results indicate that shifts in the dynamics of trees, the insects that feed on them, and the predators that feed on those insects could be altered by ongoing changes in atmospheric composition, with implications for the future health of forests.
- Enhanced Monsoon could alter Mojave Desert vegetation: Many climate models predict an enhanced monsoon in the southwestern United States, which could include additional rain in the Mojave Desert. Three years of a field experiment in the Mojave Desert, including added summer rain (three 25 millimeter events) have resulted in stimulation of growth in the dominant perennial plants. Deeper penetration into the soil of wetting fronts caused by added summer rain resulted in increased depth of root growth of several shrubs, including creosote bush. These results indicate that an enhanced future monsoon in the Southwest might change the structure and functioning of Mojave Desert scrub plant communities in favor of more deep-rooted plants capable of exploiting this additional moisture.
- Warming and increased carbon dioxide concentration accelerates succession in terrestrial ecosystem: The warmer temperatures and increased atmospheric carbon dioxide concentrations associated with urban areas, relative to upwind rural areas, was used to study effects of warming and rising carbon dioxide levels on the early stages of ecosystem secondary succession (i.e., the development of an ecosystem following a disturbance). The warming and elevated carbon dioxide levels now associated with urban Baltimore broadly reflect conditions expected about 50 years from now in rural areas. The present Baltimore conditions increased plant growth, including the growth of weedy species, and accelerated a shift from annual herbaceous species to perennial plant species, including young trees. The results indicate that warming and increasing carbon dioxide concentration may both enhance plant growth and accelerate successional processes following ecosystem disturbance in Maryland and in ecologically and climatically similar regions.
- New Ecological Research Facility Becomes Operational: A research facility at the Oak Ridge National Laboratory was established for studying the effects of atmospheric $CO_2$ enrichment, warming, and altered soil moisture on old-field ecosystems, which represent an important stage of recovery from disturbance in many ecosystems. Plants typical of old-field communities were

established within field chambers. Chamber air is modified to provide current or elevated (+300 ppm) $CO_2$ concentration in combination with near-current (+0.5 °C) or elevated (+3.2 °C) temperature. Rain is excluded from the ecosystems and water is added to maintain wet or dry soil conditions. Effects of these environmental changes on the organisms within these ecosystems, and the ecosystems themselves, will be quantified during coming years. The establishment of this research facility meets a near-term milestone of the U.S. Climate Change Science Program.

- Soil communities altered by elevated atmospheric carbon dioxide and ozone concentrations: Soil microorganisms depend on plant litter (dead plant parts) as a source of food, therefore, increases in plant litter production caused by elevated $CO_2$ and declines in litter production caused by elevated $O_3$ could alter microbial community composition and functioning. Exposure of aspen, aspen-birch, and aspen-sugar maple stands to elevated carbon dioxide resulted in greater fungal metabolism of plant litter, whereas exposure of the trees to elevated ozone eliminated this response. Molecular analysis of fungal DNA in the soils under the trees revealed that elevated carbon dioxide favored a community of litter degrading fungi that was ecologically distinct from that favored by elevated $O_3$; both differed from the fungal community under the present ambient atmosphere. Results indicate that fungal community composition and activity in soils (and perhaps biodiversity) will be modified as atmospheric concentrations of carbon dioxide and ozone continue to change.

## Detailed Justification

(dollars in thousands)

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| **Climate Forcing** | **74,346** | **78,980** | **77,831** |
| ▪ **Atmospheric Radiation Measurement (ARM) Research** | **12,243** | **13,731** | **14,765** |

In FY 2007, the principal goal of the ARM research will continue to be the development of an improved understanding of the radiative transfer processes in the atmosphere and to formulate better parameterization schemes of these processes in climate prediction models, referred to as General Circulation Models (GCMs). The increased funding will be used to support research using ARM data to develop and test cloud resolving models and other parameterization schemes and incorporate them in cloud modeling approaches such as the Multi-scale Modeling Framework. The cloud modeling approaches will then be incorporated in Atmospheric General Circulation Models to test and intercompare their performance in improving climate simulations. ARM research supports about 50 principal investigators at universities and DOE laboratories involved in studies of cloud physics and the interactions of solar and infrared radiation with water vapor, clouds, and aerosols (including black soot). University scientists form the core of the ARM science team that networks with the broader academic community, including scientists funded by NSF. Networking also occurs with the scientists at the DOE National Laboratories and with federal scientists at NASA, NOAA, and DOD. ARM scientists pursue research as individuals and as members of teams and contribute to the production of ARM data, e.g., as designers of new remote sensing instrumentation for use at ARM sites, the development and application of methods to process ARM data and produce data sets useful to researchers, as well as consumers of the data generated at the three stationary ARM sites and the new mobile ARM facility. To facilitate the knowledge transfer from the ARM program to the premier modeling centers, the ARM program also supports scientific "Fellows" at NSF's National Center for Atmospheric Research, NOAA's National Center for Environmental Prediction, and the

| | (dollars in thousands) | | |
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| | FY 2005 | FY 2006 | FY 2007 |

European Center for Medium-Range Weather Forecasting in the U.S. In addition, a model parameterization test bed that was fully implemented in FY 2004 will be continued to enable the testing and improvement of parameterization schemes and submodels by rapidly incorporating data from the ARM sites into the models to enable diagnostic tests and intercomparisons of model simulations with real world data.

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| ▪ **Atmospheric Radiation Measurement (ARM) Infrastructure** | **34,343** | **35,214** | **35,174** |

In FY 2007, the ARM infrastructure will continue to support and maintain three stationary ARM Cloud and Radiation Testbeds (CART) facilities and associated ground-based instrumentation. It will also support the maintenance, upgrading and deployment of the ARM mobile facility. It will also continue to support application of the ARM Unmanned Aerial Vehicle for use in field campaigns around the ARM facilities to provide sustained measurements at different altitudes of cloud and atmospheric properties and processes. BER will continue to operate over two hundred instruments for charactering atmospheric properties and processes and measuring solar and infrared radiation at the Southern Great Plains facility. It will also continue operations at the Tropical Western Pacific ARM facility and the North Slope facility in Alaska. The ARM program will continue to provide data to the scientific community through the ARM Archive.

The ARM data streams will continue to be enhanced periodically by additional measurements at the ARM facilities during intensive field campaigns referred to as Intensive Operational Periods (IOPs). Ranging from two weeks to two months, the campaigns bring together teams of scientists to coordinate measurements with airborne and satellite observations to measure particular processes and their effects on radiation around one of the facilities. These IOPs often involve coordinating the ground-based measurements with airborne and satellite observations. The ARM facilities have become major testbeds of research on atmospheric processes, serving as scientific user facilities for hundreds of scientists from universities and government laboratories. Both NASA and DOD, for example, have used the ARM facilities to "ground truth" measurements made with some of their satellite-based instruments. The ARM program, including the ARM UAV, will conduct a major field campaign focusing on the interactions between the land surface and the life cycle of clouds. The CCRI ARM program will continue to deploy an ARM mobile facility in selected locations that are either data poor or represent locations of opportunity for measuring effects of atmospheric conditions on the radiation balance that are currently poorly understood (e.g., direct and indirect effects of aerosols and their interactions with clouds). The primary criterion for deployment of the mobile facility is to provide needed measurements to address specific modeling needs that cannot be provided by measurements from the stationary ARM facilities. In FY 2007, the ARM mobile facility will be deployed at a site in the Arctic during the International Polar Year to study the impact of clouds, aerosols and surface characteristics on the arctic climate. Activities will be coordinated with other U.S. agencies and Arctic countries, such as Canada, Russia, and Norway. Data products will continue to be developed through collaboration with model developers.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions, and are selected through competitive, merit review processes.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Atmospheric Science** | **13,017** | **12,552** | **12,551** |

The CCSP 10-year Strategic Plan raised the priority of research dealing with the direct and indirect effect of atmospheric aerosols on climate. As a result, BER restructured the entire Atmospheric Science Program in FY 2005 to focus on research dealing with aerosol properties and processes and their effect on radiation and climate.

In FY 2007, the Atmospheric Science Program (ASP) will continue to characterize the physical, chemical, and optical properties of energy-related aerosols and their potential effects on climate. This will include laboratory studies and field research to understand aerosol formation and transformation processes and their effect on aerosol radiative properties, including the indirect effect on cloud properties and processes. Acquired data will be used to develop and test predictive parameterization schemes or models for aerosol properties and their effect on radiative transfer in the atmosphere. The ASP will also support the development of new instruments for measuring aerosol properties and processes of importance to climate. The ASP aerosol research will continue to be closely coupled and coordinated with other components of DOE's climate change research, especially the ARM and climate modeling programs. The ASP will also continue to be broadly coordinated with the climate change research in other agencies, including collaborations with NOAA, NASA, NSF, and EPA, and with the DOE Office of Fossil Energy's Airborne Fine Particulate Matter (PM) Research program. Much of the research will involve multi-agency collaboration, and university scientists will play key roles. The information is essential for improving the scientific basis for assessing the effects of energy-related emissions on climate and will contribute to the evaluation of science-base options for minimizing the impacts of energy production on climate change.

The ASP will conduct a major collaborative field campaign in FY 2007 aimed at determining the sources, chemical and physical properties and radiative properties of aerosols derived from a major urban area. In addition, data collection from the field campaign conducted downwind of Mexico City, Mexico in 2006 will be analyzed and results will be used to develop and test new schemes for modeling aerosol transformation processes, including the chemical, physical, and optical properties of aerosols and aerosol precursors emitted from this large urban area.

Research activities in this subprogram are carried out by scientists at National Laboratories, universities and private institutions and are selected through competitive and merit-review processes.

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| ▪ **Terrestrial Carbon Processes** | **11,254** | **12,480** | **13,332** |

In FY 2007, BER will continue support of the AmeriFlux program, a network of research sites that measure the net exchange of carbon dioxide, energy, and water between the atmosphere and major terrestrial ecosystems in North America. These measurements are linked to field measurement campaigns across major regions of North America that are designed to test how well point measurements of fluxes represent fluxes observed over larger areas within the same region and allow the estimate of carbon sources and sinks on a regional and eventually a national or continental basis.

The research supports the interagency Carbon Cycle Science Plan which is focused in the near term on the North American Carbon Plan that is designed to quantify the magnitude and location of the North American carbon sink. The increased funding in FY 2007 will be used to support additional

| | FY 2005 | FY 2006 | FY 2007 |
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process studies that are needed to interpret the observed variation in carbon fluxes at some of the AmeriFlux sites.

BER will also continue research to refine and test terrestrial carbon cycle models based on mechanistic representation of important carbon cycle processes and carbon accounting. The models will be used to estimate the magnitude of potential carbon sinks and sources in response to changes in environmental factors, including climate variation.

In FY 2007, BER's terrestrial carbon cycle research, as a partner in the interagency North American Carbon Program (NACP) will provide data, modeling, and analysis products from field measurements and campaigns. Data on net exchange of carbon dioxide will be produced by about 15-20 of the AmeriFlux Network sites, and these data along with information from research on fundamental mechanisms and processes will help in testing remote sensing observations and model calculations of terrestrial sources and sinks of carbon for specific region of North America.

Research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and are selected through competitive and merit-review processes.

| | FY 2005 | FY 2006 | FY 2007 |
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| ▪ **Ocean Sciences** | **1,622** | **3,130** | **136** |

Ocean sciences research is concluded. DOE has met its commitment to the scientific community to support the analysis of ocean carbon data. Analysis of ocean carbon data and modeling of ocean carbon cycling is being done by other agencies (e.g., NSF, NOAA, and NASA) eliminating the need for continuing DOE investments in these areas. Funding will be used to support one investigator to write and publish a summary article describing the major results and accomplishments of BER's ocean carbon cycle research.

| | FY 2005 | FY 2006 | FY 2007 |
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| ▪ **Information and Integration** | **1,867** | **1,873** | **1,873** |

The Information and Integration element of Climate Forcing research will continue to store, evaluate, quality assure and disseminate a broad range of climate change related data, especially data on atmospheric concentrations of greenhouse gases, industrial emissions of greenhouse gases, greenhouse gas fluxes from terrestrial systems, ocean $pCO_2$ data, and air quality data. Disseminating such data to the climate change research community for use in assessing changes in climate forcing due to increasing concentrations and emissions of greenhouse gases, for example, is an important function served by the Information and Integration element of BER's Climate Forcing research. The Carbon Dioxide Information and Analysis Center funded through BER's Information and Integration element, for example, is recognized as a World Data Center for accessing information on greenhouse gas emissions and concentrations. The Center serves a diverse set of users, including academic and laboratory scientists and policy makers globally. BER will also continue the Quality Systems Science Center for the tri-lateral (US, Mexico, Canada) NARSTO (formerly known as the North American Strategy for Tropospheric Ozone), a public partnership for atmospheric research in support of both air quality management and research on the effects of air quality on climate forcing and climate change. This Center also serves a diverse set of users, especially across North America, including both scientists and policy makers.

| | (dollars in thousands) | | |
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| | FY 2005 | FY 2006 | FY 2007 |
| **Climate Change Modeling**........................................ | **27,507** | **26,680** | **25,175** |

Model-based climate prediction provides the most scientifically valid way of predicting the response of the climate system to current and future changes in natural and human-induced forcing of the climate system over decade to century time scales. BER will continue to develop, improve, evaluate, and apply the best coupled atmosphere-ocean-sea ice-land surface models (GCMs) that simulate climate variability and over these time scales. The goal is to achieve statistically accurate forecasts of climate over regions as small as river basins using ensembles of model simulations. The ensembles will accurately incorporate the dynamic and thermodynamic feedback processes that influence climate, including clouds, aerosols, and greenhouse gas forcing. Current predictions are limited by computational resources and uncertainties in the model representations of key small-scale physical processes, especially those involving clouds, evaporation, precipitation, and surface energy exchange. BER will continue to address both the computational and scientific shortcomings through an integrated effort. Support will continue to provide climate simulations using present models that are being improved and future models that are under development. Support will continue to provide climate modelers access to the high-end computational resources needed to complete ensembles of climate simulations for modeling experiments using present and future climate models. BER will emphasize research to develop and employ information technologies that can quickly and efficiently work with large and distributed data sets of both observations and model predictions to produce quantitative information suitable for studies and assessments of climate change at regional to global scales. BER will also continue to fund the multi-institutional research consortia established in FY 2001 to further the development of comprehensive coupled GCMs for climate prediction that are of higher resolution and contain accurate and verified representations of clouds and other important climate processes. In FY 2007, BER will continue the partnerships with the Advanced Scientific Computing Research program. This includes applying the computing resources for climate simulation and continuing the improvement and development of climate model codes so they run efficiently across a wide variety of computing platforms. In addition, BER will continue to emphasize the development and application of data assimilation methods so as to quickly make use of the high-quality observational data streams from the ARM program, satellites, and other CCSP climate change programs to evaluate model performance.

In FY 2007, BER will focus on providing important input to the Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report, specifically model-based scenarios of future potential climate change to different natural and human-induced climate forcing scenarios. Support for both the CCPP-ARM parameterization testbed and CCPP university research grants that complement current SciDAC computational research for climate modeling will be reduced. The model projections generated for the Fourth IPCC Assessment Report will be further analyzed to assess how well they simulate climate dynamics and historic climate patterns and trends, including interannual climate variability and abrupt climate changes. These activities will be essential for understanding the state-of-the-science of U.S. climate modeling and uncertainties in simulating future climatic changes. BER will also continue to provide the infrastructure for evaluating the performance of major climate models and defining what changes may be needed to improve their performance. This will be done through continued support and coordination of model-data intercomparisons, the development and improvement of diagnostic tools for evaluating model performance, and the maintenance of test beds for evaluating model parameterizations.

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| | FY 2005 | FY 2006 | FY 2007 |

In FY 2007, BER's SciDAC program ($9,720,000) will continue to focus on providing models used for climate simulation and prediction. This will include the development and implementation of coupled earth system models that can simulate the interactions between the climate system and the carbon cycle, the effect of sulfate aerosols on climate, and the effect of land cover changes on climate. Efforts will also be continued to provide software engineering support for the Community Climate System Model, a code used by hundreds of researchers on many different high-end computing platforms. Research will also continue on the development of a prototype climate model of the future using new approaches to modeling climate.

The research activities in this subprogram are carried out at National Laboratories, universities, and private institutions and are selected through competitive and merit-review processes.

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| **Climate Change Response** | **25,132** | **24,986** | **23,181** |
| ▪ **Ecosystem Function and Response** | **13,896** | **12,934** | **11,583** |

In FY 2007, ecological research will continue to develop more mechanistic understanding of the scales of response of complex ecological systems to environmental changes, including identifying the underlying causal mechanisms and pathways and how they are linked, ranging from the proteomes of individual species to the whole ecosystem. The focus will be on understanding the responses of ecological systems to climatic and atmospheric changes, especially the linkages of scales in model terrestrial ecosystems containing simplified but hierarchical communities (e.g., higher plants, consumers of plant production, and microbes that decompose plant material and mineralize nutrients essential for plant growth). A key environmental factor (e.g., temperature, $CO_2$ concentration, nutrient supply) that is known to affect ecosystem functioning is experimentally manipulated and responses of individual species and the whole ecosystem will be measured at different scales, ranging from the proteome and/or genome of individual species to the entire community and ecosystem. Advanced biologically-based computational algorithms and ecosystem models will be developed to establish whether and how genomic changes (in single species, communities or whole systems) explain the responses and behavior of the entire complex ecosystem. Tools and principles developed from this research is expected to have broad generality and eventual application to problems in ecological risk assessment, carbon sequestration, environmental restoration and cleanup, and early detection of ecological responses to climatic and atmospheric changes and other environmental factors.

In FY 2007, BER will focus on supporting experimental research at the four Free-Air Carbon Dioxide Enrichment (FACE) sites located at Duke University (North Carolina), Rhinelander, Wisconsin, Oak Ridge, Tennessee, and Mercury Nevada on the Nevada Test Site. Support for other on-going or new experimental studies will be reduced. The on-going experiments will improve understanding of the direct effects of experimentally elevated carbon dioxide and other atmospheric changes (such as elevated ozone) on the structure and functioning of various terrestrial ecosystems, including their capacity to sequester carbon at the elevated level of atmospheric carbon dioxide. Emphasis will continue to be on understanding the cause of differential responses of plant species that may impact plant competition, succession, and productivity of terrestrial ecosystems. Research will also continue to explore changes over time in the effects of elevated atmospheric carbon dioxide

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

concentrations on net primary productivity and the allocation of fixed carbon to soil and living biomass in either plant roots or aboveground stems and branches or both.

The long-term experimental investigation of altered precipitation on an eastern deciduous forest at Oak Ridge, Tennessee will continue to improve understanding of the direct and indirect effects of changes in the annual average precipitation amount on the structure and functioning of this forest. Both the four FACE facilities and the altered precipitation experiment at Oak Ridge represent scientific user facilities that have attracted scientists from both academic institutions and government laboratories who use these facilities to test scientific hypotheses related to ecosystem responses to climatic and atmospheric changes.

| | | | |
|---|---|---|---|
| ▪ **Free Air Carbon Enrichment (FACE) Facility** | **5,697** | **5,796** | **5,400** |

In FY 2007, BER will continue to provide support to maintain and operate the four up-graded FACE facilities located at Rhinelander, Wisconsin, Mercury, Nevada on the Nevada Test Site, Duke Forest and Duke University, North Carolina, and Oak Ridge, Tennessee. The funding decrease is a result of completion of the upgrade of the FACE facilities. These four experimental field facilities provide semi-controlled environments for use by investigators to test hypotheses about the direct and indirect effects of elevated carbon dioxide and/or other gases on the structure and functioning of different terrestrial ecosystems. Funds for the FACE facility will continue to be used to maintain the four experimental facilities, including the purchase of carbon dioxide, the purchase of electricity to operate the facility, the logging of data on facility operations, and, when necessary, replacement of instruments, control systems and materials that are essential for continued, safe operation of the facilities. It includes support of staff required to operate and maintain the facilities so as to ensure they meet the experimental requirements of users. The four FACE facilities and scientific user facilities attract scientists from academic institutions, government laboratories, other countries, and other agencies to test specific hypothesis and to collect data required to answer specific scientific questions.

| | | | |
|---|---|---|---|
| ▪ **Integrated Assessment** | **4,118** | **4,830** | **4,772** |

The Integrated Assessment Program, with a strong academic involvement, will continue to support research to improve methods and models that can provide better estimates of the costs and benefits of possible actions to mitigate global climate change. The goal is to improve the integrated assessment models to include several greenhouse gases, and international trading of emission permits. Model improvements are needed to better represent the efficiency gains and losses of alternative emission reduction plans, including market adjustments to interregional differences among relative energy prices, regulations, and production possibilities in the international arena.

The Integrated Assessment Program will support research to develop internally consistent sets of scenarios that can be used for national-scale decision making. The scenarios will be evaluated in selected integrated assessment models also funded by the program.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| | (dollars in thousands) | | |
| ▪ **Education** | **1,421** | **1,426** | **1,426** |

BER's Global Change Education Program will continue to support DOE-related research in climate change for both undergraduate and graduate studies through the DOE Summer Undergraduate Research Experience (SURE) and the DOE Graduate Research Environmental Fellowships (GREF). Both the GREF and the SURE provide students with the opportunity to propose and conduct research that is of interest to them and relevant to DOE's climate change research. Their research is conducted under a mentor of their choice at either a university or a DOE laboratory. The SURE continues to be a magnet for highly qualified undergraduates most of whom have gone on to graduate school to study in fields directly related to what they did under SURE. Similarly students in the GREF program have received graduate degrees and many have stayed in the field and initiated their own research related to climate change. Both SURE and GREF will be continued in FY 2007 to support climate change research by undergraduate and graduate students and thereby contribute to the training of students for future careers in climate change research.

| | | | |
|---|---|---|---|
| **Climate Change Mitigation** | **8,550** | **6,947** | **5,014** |

Ocean carbon sequestration research is concluded in FY 2006. This is due to adverse effects on deep ocean biology and chemistry of injecting a relatively pure stream of carbon dioxide into the deep ocean as a possible strategy for sequestering carbon dioxide separated from fossil fuel power plants and industrial stack gases.

In FY 2007, BER's carbon sequestration research will focus only on terrestrial carbon sequestration. Research will continue on studies to identify and understand the biological and environmental processes (e.g., carbon assimilation, retention and storage) that limit or constrain carbon sequestration in terrestrial ecosystems and to develop approaches (e.g., genetic selection, microbial manipulation, and soil carbon management) for overcoming such limitations to enhance sequestration long-term storage pools in terrestrial vegetation and soils. It will also continue to support research needed to understand and assess the potential environmental implications of purposeful enhancement of carbon sequestration in terrestrial ecosystems.

| | | | |
|---|---|---|---|
| **SBIR/STTR** | **—** | **3,936** | **3,708** |

In FY 2005 $3,476,000 and $418,000 were transferred to the SBIR and STTR programs, respectively. FY 2006 and FY 2007 amounts are the estimated requirements for continuation of the programs.

| | | | |
|---|---|---|---|
| **Total, Climate Change Research** | **135,535** | **141,529** | **134,909** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Climate Forcing** | |
| ▪ The ARM research increases to support research using ARM data to develop and test cloud resolving models and other parameterization schemes and incorporate them in cloud modeling approaches such as the Multi-scale Modeling Framework. The cloud modeling approaches will then be incorporated in Atmospheric General Circulation Models to test and intercompare their performance in improving climate simulations. | +1,034 |
| ▪ The ARM infrastructure remains at near FY 2006 levels. | -40 |
| ▪ Atmospheric Sciences is held at FY 2006 levels. | -1 |
| ▪ Terrestrial Carbon Processes research increases to support additional process studies that are needed to interpret the observed variation in carbon fluxes at some of the AmeriFlux sites. | +852 |
| ▪ Ocean Sciences research is concluded. DOE has met its commitment to the scientific community to support the analysis of ocean carbon data. Analysis of ocean carbon data and modeling of ocean carbon cycling is being done by other agencies (e.g., NSF, NOAA, and NASA) which negate the need for continuing DOE investments in those efforts. | -2,994 |
| **Total, Climate Forcing** | **-1,149** |
| **Climate Change Modeling** | |
| ▪ Climate Modeling - Support for the Climate Change Prediction Program-ARM Parameterization Testbed will be scaled back because the increased funding for ARM science will allow it to cover most of the costs of testing the performance of parameterization schemes (e.g., cloud models) in climate models. In addition, the Climate Change Prediction Program investments will be scaled back and reduced to projects that complement SciDAC projects, thus focusing on analysis of long-term observational data and climate model simulation data sets to yield new insights into climate variability and change. Support for university grants that complement the current SciDAC computational research for climate modeling will be reduced because the SciDAC projects at DOE labs are considered adequate to meet existing programmatic needs. | -1,505 |
| **Climate Change Response** | |
| ▪ Ecosystem Function and Response decreases. Support for major experimental studies to quantify the response of terrestrial ecosystems to climatic and atmospheric changes will be reduced to support higher priority programs within BER. This will delay the initiation of new experimental studies and the production of data needed to produce and test models for simulating the response of some major ecological systems to climatic changes. | -1,351 |

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| ▪ FACE user facility funding decreases as the upgrade of the facility has been completed. | -396 |
| ▪ Integrated Assessment is held at FY 2006 levels. | -58 |
| **Total, Climate Change Response** | **-1,805** |
| **Climate Change Mitigation** | |
| ▪ Carbon Sequestration research - Ocean Carbon Sequestration research is concluded. Because of the adverse effects of deep ocean disposal of $CO_2$ on ocean biology and ecology, and the ineffectiveness and potential risks to the ecology of the ocean of large-scale iron fertilization, neither ocean sequestration option is currently considered environmentally acceptable or viable. Hence, there is no need for continuing research on ocean sequestration as a potential option for helping to mitigate the increase in atmospheric $CO_2$ concentrations. | -1,933 |
| **SBIR/STTR** | |
| ▪ SBIR/STTR reduced due to research program reductions. | -228 |
| **Total Funding Change, Climate Change Research** | **-6,620** |

## Environmental Remediation

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Environmental Remediation | | | |
| Environmental Remediation Sciences Research | 61,435 | 52,270 | 50,479 |
| Facility Operations | 39,140 | 39,190 | 44,453 |
| SBIR/STTR | — | 2,284 | 2,264 |
| Total, Environmental Remediation | 100,575 | 93,744 | 97,196 |

### Description

The mission of the Environmental Remediation subprogram is to deliver the scientific knowledge, technology, and enabling discoveries in biological and environmental research needed to underpin the Department of Energy's mission for environmental quality.

### Benefits

The fundamental research supported in this subprogram will reduce the costs, risks, and schedules associated with the cleanup of the DOE nuclear weapons complex; extend the frontiers of methods for remediation; discover the fundamental mechanisms of contaminant transport in the environment; and develop cutting edge molecular tools for investigating environmental processes. This research also will provide fundamental knowledge that applies to a broad range of remediation problems, including avoidance of environmental hazards for future nuclear energy options.

### Supporting Information

Research priorities for the Environmental Remediation Sciences subprogram include defining and understanding the processes that control contaminant fate and transport in the environment and providing opportunities for use, or manipulation of natural processes to alter contaminant mobility. The subprogram also is responsible for operation of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL). This national user facility provides advanced molecular tools to the scientific community to address critical environmental issues including:  environmental remediation, contaminant fate and transport in the environment, biology and genomics applications in the environment, atmospheric science and physical chemistry.

Within the subprogram, the EMSL budget is to be increased to maintain operations at full capacity. Reductions in Environmental Remediation Sciences research funding will result in the termination of research on high-level waste, including waste storage tanks. Currently funded projects in this area of research will be terminated. This will eliminate SC efforts to develop science-based alternatives for the closure and long-term stewardship of high-level waste and waste storage tanks. As a result of ongoing prioritization by BER, research emphasis within the Environmental Remediation Sciences subprogram is being focused on issues of subsurface cleanup. The nature of the scientific questions and the timelines associated with those questions are better suited to the basic science mission of Environmental Remediation Sciences than are those of high level waste.

The Environmental Remediation Sciences subprogram research activities were integrated in FY 2006 based on recommendations of a BERAC Committee of Visitors (COV) review. The COV report was supportive of the subprogram and the approach to selecting and funding research projects. The COV found that Environmental Remediation Sciences activities were well-focused on the key science needs for DOE clean-up. The COV supported previous recommendations to expand opportunities for field-based research within the subprogram.

The Environmental Remediation subprogram will develop a fundamental understanding of biological, chemical and physical phenomena across a range of scales up to and including the field scale. The resulting knowledge and technology will assist DOE's environmental clean-up and stewardship missions by developing: a more comprehensive understanding of contaminant fate and transport, *in situ* remediation technologies, subsurface characterization techniques, and performance monitoring of remedial technologies. This will be accomplished by soliciting and funding a range of projects from lab-based, single investigator research to complex, multidisciplinary, large-scale research projects that evaluate processes relevant to the environment at the field scale. This broad-based, tiered approach responds to the recommendations of the BERAC Environmental Remediation Sciences subcommittee and the COV review. The recently integrated research program is designed to respond to the BER long-term environmental remediation measure "…to provide sufficient scientific understanding to allow a significant fraction of DOE sites to incorporate coupled biological, chemical and physical processes into decision making for environmental remediation."

Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes.

**FY 2005 Accomplishments**

- Field Research Leads to Advances in Understanding the Role of Microbes in Contaminant Fate & Transport: Following recommendations of its BERAC subcommittee and a Committee of Visitors, the Environmental Remediation Sciences subprogram is expanding field-based research. Current field research helped to establish the potential for subsurface microorganisms to immobilize contaminant metals and radionuclides *in situ*. Researchers at the Old Rifle Uranium Mill Tailings Remedial Action (UMTRA) site are using advanced DNA and mRNA techniques to link gene expression of subsurface metal-reducing bacteria to the bioremediation of uranium. The results show that increases in gene expression levels can be used to quantitatively model microbial metabolism *in situ*. Thus, gene expression techniques may be used to better design natural and enhanced bioremediation technologies. Researchers at the Hanford site have successfully tested a commercially available product that enhances the activity of metal-reducing microorganisms to immobilize chromium in the subsurface. Work at the Field Research Center (FRC) at the Oak Ridge site is demonstrating an *in situ* remediation process that manipulates subsurface conditions to make uranium available for consequent reduction and immobilization by microorganisms. Sequencing efforts at the JGI will provide the first example of a complete set of sequenced genomes of a complex subsurface microbial community (Oak Ridge FRC). These results should allow a comprehensive description of the genetic potential of a subsurface microbial community. The incorporation of seismic and electrical surveys during *in situ* stimulation of microbial communities indicated that stimulated changes in the subsurface could be monitored over time by surface measurements, markedly reducing the need for recovery of expensive cored material from the subsurface.

- Grand Challenges in Environmental Molecular Sciences: The Environmental Remediation Sciences subprogram, in collaboration with Pacific Northwest National Laboratory (PNNL), has implemented a Grand Challenges concept at the Environmental Molecular Sciences Laboratory (EMSL). EMSL has launched two scientific Grand Challenges that will bring together some of the world's leading environmental molecular scientists to study fundamental questions in membrane biology and biogeochemistry that underlie issues critical to DOE and the Nation. Grand Challenges engage multi-institutional and multidisciplinary teams to address complex, large-scale scientific and engineering problems with broad scientific and environmental or economic impacts by using multiple experimental and computational capabilities within the EMSL. Scientists from more than twenty universities and research institutions worldwide are focused on the first EMSL Grand Challenges in biogeochemistry and membrane biology. The EMSL Grand Challenge in Biogeochemistry is led by PNNL scientists and is examining a key feature of the interface between the biosphere and the geosphere: how microorganisms regulate energy, electron and proton fluxes between cells and mineral solids present in soils and subsurface sediments. The research is expected to have broad implications for contaminant transport in the environment and remediation, corrosion, mineral formation and for understanding global biogeochemical cycles. The EMSL Grand Challenge in Membrane Biology is led by university scientists and is directed toward the fundamental changes that occur in membrane processes in Cyanobacteria due to changes in the surrounding environment. This investigation of one of the most abundant groups of microorganisms on earth is expected to make significant contributions to the harvesting of solar energy, global carbon sequestration, nutrient metal acquisition, and hydrogen production in marine and freshwater ecosystems.
- High-level Waste: The high-level radioactive waste program continued with 75 projects in FY 2005, addressing key scientific issues in characterization of tank wastes, separation and processing of components of the wastes that have been removed from the storage tanks, and assessing the stability of waste storage forms. This research already demonstrated direct value to the Environmental Management (EM) cleanup program through, for example, reduction of foaming problems that disrupted waste processing, and through development of novel extraction agents for removal of strontium from waste mixtures. Each of these accomplishments resulted in large savings of both cost and time by solving otherwise intractable problems. Current research is directed at overcoming a number of major obstacles in the cleanup process, including finding means of reducing the volumes of alkaline tank waste and development of green separation technologies that minimize residue from processing of high level radioactive wastes.
- New Efforts in the Environmental Molecular Sciences: Researchers at the DOE/National Science Foundation (NSF) co-funded Environmental Molecular Science Institutes (EMSIs) are providing fundamental insights into reactions occurring at the water-mineral interface and within microbial biofilms at mineral surfaces, issues critical to prediction of contaminant fate and transport as well as to development of new remediation concepts. Researchers at the Stanford University EMSI are continuing to probe the fundamental structure of liquid water. Previous research by this group was recently featured as one of the top ten science stories of 2004 by *Science* magazine. Investigations at the Penn State University EMSI are documenting the rates of environmentally important reactions occurring across a variety of scales within the subsurface. An American Chemical Society symposium led by Penn State EMSI researchers highlighted the issues involved in scaling geochemical reactions occurring at the sub-nanometer scale to processes occurring at the field scale (meters to kilometers). These researchers also have developed a computer model that begins to describe changes in subsurface pore structure due to mineral precipitation in groundwater—a key issue for contaminant immobilization technologies. Researchers at the Stony Brook University EMSI

continue to probe geochemical reactions that lead to the sequestering of contaminants, such as arsenic and radionuclides, at mineral surfaces and immobilization of contaminants in subsurface environments.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Environmental Remediation Sciences Research** | **61,435** | **52,270** | **50,479** |
| ▪ **Environmental Remediation Sciences Research** | **56,892** | **45,727** | **43,936** |

The Environmental Remediation Sciences Research activity will address critical questions of fundamental environmental remediation science at the interfaces of biology, chemistry, geology and physics. Research results will provide the scientific foundation for the solution of key environmental challenges within DOE's cleanup mission at scales ranging from molecular to the field, including issues of fate and transport of contaminants in the environment; novel strategies for *in situ* remediation; and long-term monitoring of remediation strategies.

The research activity will support a tiered set of projects that range from relatively small, specialized, single investigator, laboratory-based research projects to complex, multidisciplinary, large-scale research projects that evaluate processes relevant to the environment at the field scale. The overall focus and integration strategy will center on field research since the ultimate goal of the Environmental Remediation Sciences subprogram is the development of science-based remediation strategies and a conceptual understanding of environmental processes that can be implemented to solve existing environmental problems. In addition to research on the environmental processes that control contaminant transport, this activity will develop new tools for measuring and characterizing the broad range of biological, environmental, and geophysical parameters associated with the behavior of contaminants in the environment. This broad-based, tiered approach responds to recommendations of the BERAC Environmental Remediation Sciences subcommittee and a Committee of Visitors review.

This integrated research effort will lead to the development of improved models to predict the transport of contaminants in the environment and then to validate those predictions using field data. Knowledge of the factors controlling contaminant mobility in the environment is essential to understand the fate of contaminants, before, during, and after remediation, and is a necessary step toward the BER long-term measure for environmental remediation. Funding reductions in FY 2006 have delayed plans to initiate new field-based research aimed at achieving that goal. These new efforts are now planned for initiation in FY 2007 and will complement ongoing work at the Oak Ridge Field Research Center (FRC), the Old Rifle UMTRA site and the Hanford site. This expanded field-based research will allow scientists to evaluate concepts and hypotheses under a variety of geochemical conditions. The expanded field efforts will have broad applicability to current research programs on heavy metal and radionuclide contamination as well as to the DOE clean-up mission. These new activities also will emphasize the need for coordination between experimentation and computer simulation as critical components of both experimental design and model development.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

The expanded field research activities will be used to evaluate and validate the results of laboratory-based science and predictive modeling efforts.

This newly integrated research activity will continue to foster interdisciplinary research and be more responsive to new knowledge and to advanced computational and analytical tools that emerge from research at the EMSL, the synchrotron light sources, and from within the GTL program in support of DOE's clean-up mission.

BER participation in SciDAC will provide an opportunity for subsurface and computational scientists to develop and improve methods of simulating subsurface reactive transport processes on "discovery class" computers. The intent is to explore potential advantages that high-end computing can bring to the understanding of optimal model complexity, the scalability of biogeochemical reactions, model abstraction methods, sources of uncertainty, parameter estimation and characterization measurements as input in subsurface reactive transport modeling.

In FY 2007 reductions in Environmental Remediation Sciences subprogram research funding will result in termination of research in high-level waste, including waste in storage tanks. Currently funded projects in this area of research will be terminated. This will eliminate SC efforts to develop science-based alternatives for the closure and long-term stewardship of high-level waste and waste storage tanks. As a result of ongoing prioritization by BER, research emphasis within the Environmental Remediation Sciences subprogram is being focused on issues of subsurface cleanup. The nature of the scientific questions and the timeliness associated with those questions are better suited to the basic science mission of Environmental Remediation Sciences than are those of high level waste. The Environmental Remediation Sciences research subprogram will narrow its research efforts to focus on subsurface science in support of its long-term measure for environmental cleanup.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **General Purpose Equipment (GPE)**.............. | **1,659** | **403** | **403** |

GPE funding will continue to provide general purpose equipment for Pacific Northwest National Laboratory (PNNL) and Oak Ridge Institute for Science and Education (ORISE) such as information system computers and networks, and instrumentation that supports multi-purpose research.

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|
| ▪ **General Plant Projects (GPP)**......................... | **2,884** | **6,140** | **6,140** |

GPP funding is continued for minor new construction, other capital alterations and additions, and for buildings and utility systems, such as replacing piping in 30- to 40-year old buildings, modifying and replacing roofs, and HVAC upgrades and replacements. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and meeting the requirements for safe and reliable facilities operation. This activity includes stewardship GPP funding for PNNL and for ORISE. The total estimated cost of each GPP project will not exceed $5,000,000.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Facility Operations** | **39,140** | **39,190** | **44,453** |
| ▪ **EMSL Operating Expenses** | **31,958** | **33,702** | **35,649** |

The EMSL is a scientific user facility located at the Pacific Northwest National Laboratory focused on conducting interdisciplinary, collaborative research in molecular-level environmental science. Operating funds are used for: staff support for users; maintenance of instruments and buildings; utilities; environment, safety and health compliance activities; and communications. With over 55 leading-edge instruments and a supercomputer system, the EMSL annually supports approximately 1,600 users. The core EMSL science team networks with the broader academic community as well as with DOE National Laboratories and other agencies. EMSL users have access to unique expertise and instrumentation for environmental research, including a Linux-based supercomputer; a 900 MHz nuclear magnetic resonance (NMR) spectrometer that highlights a suite of NMRs in EMSL; a collection of mass spectrometers, including an 11.5 Tesla high performance mass spectrometer; laser desorption and ablation instrumentation; ultra-high vacuum scanning, tunneling and atomic force microscopes; and controlled atmosphere environmental chambers.

In FY 2007 EMSL operations funding is increased to enhance user facility operations and increase services to users.

| | | | |
|---|---|---|---|
| ▪ **General Plant Projects (GPP)** | **3,200** | **—** | **—** |

The GPP (TEC $4,450,000) for EMSL's Molecular Science Computing Facility (MSCF) adds approximately 4,000 sq. ft of additional space. The additional MSCF space is needed to meet the demand for new data storage systems due to the volume of data being generated by EMSL's high-throughput mass spectrometer, NMR, and other systems. Design of this project is in progress and is planned for completion in FY 2006.

| | | | |
|---|---|---|---|
| ▪ **Capital Equipment** | **3,982** | **5,488** | **8,804** |

Capital equipment support for the EMSL enables instrument modifications needed by collaborators and external users of the facility as well as the ability to make upgrades to existing instrumentation and to provide additional capabilities in order to maintain EMSL capabilities for environmental molecular scientific research. In FY 2007 increased capital equipment funds will be used to upgrade and refresh critical analytical capabilities in the areas of surface analytics (e.g., x-ray spectroscopy, Auger electron spectroscopy, secondary ion spectroscopy); increase capacity and throughput in proteomics (additional mass spectrometers) and high-field nuclear magnetic resonance spectroscopy (additional conventional and customized cryoprobes and consoles); increase electronic data storage capacity for data archiving of spectroscopic and proteomic output, and refurbish and replace aging support equipment (e.g,. turbopumps and laser systems, cryostats).

| | | | |
|---|---|---|---|
| **SBIR/STTR** | **—** | **2,284** | **2,264** |

In FY 2005 $2,316,000 and $278,000 were transferred to the SBIR and STTR programs, respectively. FY 2006 and FY 2007 amounts are the estimated requirements for continuation of the programs.

| | | | |
|---|---|---|---|
| **Total, Environmental Remediation** | **100,575** | **93,744** | **97,196** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Environmental Remediation Sciences Research** | |
| ▪ Reductions in Environmental Remediation Sciences research funding will terminate research on high-level waste, including waste storage tanks. Currently funded projects in this area will be terminated. This will eliminate SC efforts to develop science-based alternatives and understanding for the closure and long-term stewardship of high-level waste and waste storage tanks. As a result of ongoing prioritization by BER, research emphasis within the Environmental Remediation Sciences subprogram is being focused on issues of subsurface cleanup. The nature of the scientific questions and the timelines associated with those questions are better suited to the basic science mission of Environmental Remediation Sciences than are those of high level waste. | -1,791 |
| **Facility Operations** | |
| ▪ In FY 2007, EMSL operations funding is increased to maintain existing levels of user service | +1,947 |
| ▪ In FY 2007, funding for EMSL capital equipment increases. Increased capital equipment funds will be used to upgrade and refresh critical analytical capabilities in the areas of surface analysis techniques; functional genomics analysis and high-field nuclear magnetic resonance spectroscopy. These funds will also increase electronic storage capacity within EMSL for archiving spectroscopic and functional genomics data by allowing refurbishment or replacement of aging archival support equipment | +3,316 |
| **Total, Facility Operations** | **+5,263** |
| **SBIR/STTR** | |
| ▪ SBIR/STTR decreases with reduction in research. | -20 |
| **Total Funding Change, Environmental Remediation** | **+3,452** |

## Medical Applications and Measurement Science

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Medical Applications and Measurement Science | | | |
| Medical Applications | 117,858 | 138,576 | 13,608 |
| Measurement Science | 4,066 | — | — |
| SBIR/STTR | — | 3,987 | 392 |
| Total, Medical Applications and Measurement Science | 121,924 | 142,563 | 14,000 |

### Description

The mission of the Medical Applications and Measurement Science subprogram is to deliver the scientific knowledge and discoveries that will lead to new radio-isotopically based diagnostic and therapeutic tools, non-invasive medical imaging technology, and bioengineering solutions to critical medical problems.

### Benefits

The basic research supported by the subprogram leads to new diagnostic and therapeutic technologies and reagents for the medical community that impact medical imaging and cancer treatment. The research also leads to the development of new medical devices such as neural prostheses, e.g., an artificial retina, that improve quality of life for affected patients.

### Supporting Information

The modern era of nuclear medicine is an outgrowth of the original charge of the Atomic Energy Commission (AEC), "to exploit nuclear energy to promote human health." From the production of a few medically important radioisotopes in 1947, to the development of production methods for radiopharmaceuticals used in standard diagnostic tests for millions of patients throughout the world, to the development of ultra-sensitive diagnostic instruments, e.g. the PET (positron emission tomography) scanner, the Medical Applications program has led and continues to lead the field of nuclear medicine.

Today the subprogram seeks to develop new imaging technologies and new applications of radiotracers in diagnosis and treatment driven by the latest concepts and developments in genomic sciences, structural and molecular biology, computational biology, and instrumentation. Research capitalizes on the National Laboratories' unique resources and expertise in biological, chemical, physical, and computational sciences for technological advances related to human health. The expertise of the National Laboratories in micro-fabrication, micro-electronics, material sciences, and computer modeling provides the capability to develop intelligent micro-machines (e.g., the artificial retina) that interface with the brain to overcome disabilities and novel biomedical sensors with a broad range of biomedical applications including neural prostheses, such as the artificial retina.

Coordination with the National Institutes of Health (NIH) is provided through joint participation of NIH research staff and management on BERAC Subcommittees, and NIH technical staff participation on BER merit review panels to reduce the possibility of undesirable duplications in research funding. DOE and NIH also organize and sponsor workshops in common areas of interest, for example: a joint workshop on Optical and X-ray Imaging, and Nanomedicine. Members of the Medical Sciences subprogram staff are formal members of the National Cancer Advisory Board, the BioEngineering Consortium (BECON) of NIH Institutes, and are on critical committees of the recently established National Institute of Bioimaging and Bioengineering (NIBIB). Program staff also participate in interagency activities such as the Multi Agency Tissue Engineering Science (MATES) working group that includes representatives of seven agencies and the Office of Science Technology Policy.

The Medical Applications and Measurement Science subprogram continues a substantial involvement of academic scientists along with the scientists at the National Laboratories.

Periodic retrospective analysis will be employed to evaluate the accumulation of knowledge and validate specific outcomes. This program was examined as part of a BERAC review of the entire BER program in FY 2001. The next scheduled comprehensive review of the Medical Applications and Measurement Science subprogram by a BERAC COV will be in FY 2006.

**FY 2005 Accomplishments**

- Progress in Helping the Blind to See: The DOE Artificial Retina Program (ORNL; SNL; LANL; ANL; LLNL; University of Southern California; UC, Santa Cruz; North Carolina State; and Second Sight Corp.) has made significant progress in the roadmap to developing a device to restore vision to people suffering from retinal blindness. Six blind patients have been implanted with a 16-electrode device. They are now able to recognize moving light, discriminated light from dark, and discern large objects. A sixty electrode device is completing animal testing and will be implanted in 2006. Design for a 256 electrode device has been completed and construction is underway.
- Smaller, More Versatile PET Scanners: BNL has completed a prototype mobile PET scanner ("the rat cap") which will record images in the awake animal. The mobile PET will be able to acquire positron-generated images in the absence of anesthesia-induced coma and correct for motion of the animal. The long-term goal is to develop PET instrumentation able to diagnose neuro-psychiatric disorders in children.
- Ultra-high performance Hybrid Imaging Instrumentation Developed: Scientists at the Thomas Jefferson National Accelerator Facility have built a small-animal imaging device that is an ultra-high performance gamma camera detector combined with an optical detector. The instrument is a high resolution hybrid tomographic system for small animals and is capable of producing 3 dimensional images of the distribution of both radiotracers and fluorescent/bioluminescent molecules. It will achieve a remarkable spatial resolution of under 0.5mm.
- Highest Resolution PET scanner Developed: Scientists at the LBNL have developed the world's most sensitive PET scanner. The instrument is 10-times more sensitive than a conventional PET scanner. The instrument became operational in 2005.
- Imaging Gene Expression in Cancer Cells: Images of tumors in whole animals which detect the expression of three cancer genes were accomplished for the first time by investigators at Thomas Jefferson University and the University of Massachusetts Medical Center. The three cancer genes probed were CCND1, MYC, and KRAS. This advanced imaging technology will lead to the detection of cancer in human using cancer cell genetic profiling.
- Modeling Radiation Damage to the Lung: Treatment of thyroid disease and lymphomas using radioisotopes can cause disabling lung disease. Investigators at Johns Hopkins University have developed a Monte Carlo model that can be used to determine the probability of lung toxicity and be

incorporated into a therapeutic regimen. This model will optimize the dose of radioactivity delivered to cancer cells and avoid untoward effects on the lung.

- New radiopharmaceuticals with Important Clinical Applications: The DOE radiopharmaceutical science program has developed a number of innovative radiotracers for the early diagnosis of neuro-psychiatric illnesses. Three agents were developed at the University of California at Irvine. One agent localizes to beta amyloid in the brain plaques found in Alzheimer's Disease. A new nicotine receptor imaging agent, 18F-nifrolidine has a high affinity for targets in the diagnosis and understanding of Alzheimer's Disease and schizophrenia. A new serotonin receptor imaging agent, 18F-mefway, will be useful in the diagnosis of depression and anxiety disorders.
- Rapid Preparation of Radiopharmaceuticals for Clinical Use: The preparation of radiohalogenated pharmaceuticals for use in Nuclear Medicine is a formidable task. The DOE sponsored program at the University of Tennessee has developed a totally new method for preparing radiopharmaceuticals by placing a boron-based salt at the position that will be occupied by the radiohalogen. The salt is simply mixed with a radiohalogen and the desired product decanted or filtered from the salt-like starting materials. The method has been used to prepare a variety of cancer-imaging agents
- Brain Pathway in Obesity Uncovered: Using highly-specific radiotracers as molecular probes, BNL researchers discovered a deficiency in the reward circuits in the brains of obese individuals that are similar to abnormalities observed in drug abusers. This suggests that obese individuals are overeating to compensate for a deficiency in the dopamine system in the brain which regulates the reward system. These results may be useful in developing strategies for the treatment of obesity.
- Understanding Nicotine Addiction: BNL researchers have developed a new radiopharmaceutical agent to image the brain nicotine system and have used this tracer to show striking images of nicotine binding sites in the human brain. The new radiotracer is being used to understand the molecular basis of nicotine addiction and to devise smoke-ending strategies.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **Medical Applications** ............................................ | **117,858** | **138,576** | **13,608** |
| ▪ **Medical Applications** ...................................... | **38,735** | **13,480** | **13,608** |

In FY 2007, BER supports basic research that builds on unique DOE capabilities in physics, chemistry, engineering, biology, and computational science. It supports fundamental imaging research, maintains core infrastructure for imaging research and development, and develops new technologies to improve the diagnosis and treatment of psycho-neurological diseases and cancer and the function of patients with neurological disabilities, such as blindness and paralysis. BER research develops new metabolic labels and imaging detectors for medical diagnosis; tailor-made radiopharmaceutical agents for treatment of inoperable cancers; and the capabilities to more accurately determine the structure and behavior of cells and tissues, information needed to engineer more effective or specific drugs. BER utilizes the resources of the National Laboratories in material sciences, engineering, microfabrication and microengineering to fund development of unique neuroprostheses and continue to develop construction of an artificial retina to restore sight to the blind. DOE's clinical goal for the artificial retina project is to develop the technology and construct a

| | FY 2005 | FY 2006 | FY 2007 |
|---|---|---|---|

(dollars in thousands)

1,000+ electrode intraocular device that will allow a blind person to read large print, recognize faces, and move around without difficulty.

The research activities in this subprogram are principally carried out at National Laboratories and are selected through competitive and merit-reviewed processes.

| | | | |
|---|---|---|---|
| ▪ **Congressionally Directed Activities**................. | **79,123** | **125,096** | **—** |

Congressional direction was provided in FY 2005 for a science building at Waubonsee Community College in Illinois; digital playback hardware and software for Recording for the blind and dyslexic; All Children's Hospital in Florida; Eckerd College in Florida; Applied Research and Technology Park electrical and communication infrastructure improvements in Springfield, Ohio; a Multiple Sclerosis, Alzheimer's, Parkinson's, Lou Gehrig's Imaging System at the Cleveland Clinic in Ohio; Duchenne Muscular Dystrophy research-related equipment at Children's National Medical Center in the District of Columbia; Duchenne Muscular Dystrophy research-related equipment at the University of Washington-Seattle; the Northeast Regional Cancer Center in Scranton, Pennsylvania; Ohio State University for environmental research in cooperation with Earth University; the University of Akron, Ohio, Polymer Center; the Ohio Northern University, Ada, Ohio, Science and Pharmacy Building; the Alabama A&M University; University of Texas at Arlington optical medical imaging equipment; the Missouri Alternative and Renewable Energy Technology Center, Crowder College; the San Antonio, Texas, Cancer Research and Therapy Center; the University of South Alabama Cancer Center; the Virginia Commonwealth University Massey Cancer Center; the Saint Francis Hospital, Delaware, Cardiac Catheterization Lab; the Jacksonville University Environmental Science Center; the Houston, Texas, Alliance for Nanohealth; the Virginia Science Museum; the Polly Ryon Memorial Hospital, Texas; the St. Thomas University Minority Science Center, Miami, Florida; Project Intellicare, Roseville, California; the Virginia Polytechnic Institute Center for High-Performance Learning Environment; Georgia State University; the Michigan Research Institute for life science research; the University of Arizona Environment and Natural Resources Phase I1 Facility; the Children's Hospital of Illinois ambulatory care project; the Loma Linda University, California, Medical Center synchrotron expansion; the University of Dubuque, Iowa, Environmental Science Center; the Ball State University, Indiana, Bioenergetics Research Initiative; the Clearfield Area School District, Pennsylvania, Energy Initiative; Digital Cardiology equipment at Children's Hospital and Research Center, Oakland, California; the National Childhood Cancer Foundation; the Roswell Park Cancer Institute, New York, Center for Genetics and Pharmacology; Bucknell University, Pennsylvania, Materials Science Laboratory; the Science Center at Mystic Seaport, Connecticut; the Saratoga Hospital, New York, radiation therapy center; the San Joaquin Community Hospital, Bakersfield, California; the Syracuse University, New York, Environmental Systems Center; the University of Tennessee Sim Center; the St. Mary's Hospital, Kankakee, Illinois; the Derby Center for Science and Mathematics at Lyon College in Arkansas; the Rush Presbyterian St. Lukes Medical Center in Illinois; Medical Research and Robotics at the University of Southern California; the Advanced Building Efficiency Testbed at Carnegie Mellon University; DePaul University Biological Sciences; the Philadelphia Educational Advancement Alliance; Northwestern University Institute of Bioengineering and Nanoscience in Medicine; the Rensselaer Polytechnical Institute Center for Bioscience; St. Peter's Biotechnical Research in New Jersey; the Berkshire Environmental Center in Massachusetts; the Center for the Environment at the University of

(dollars in thousands)

| FY 2005 | FY 2006 | FY 2007 |
|---|---|---|

Massachusetts; technical upgrades at St. Joseph Hospital in Arizona; the Center for Science at the University of San Francisco in California; Augsburg College in Minnesota; the Bronx Community Center for Sustainable Energy; Marquette General Hospital in Marquette, Michigan; the Illinois-Indiana Super-Grid Program connecting Argonne National Laboratory and Purdue and Notre Dame Universities; the Purdue Calumet Water Environmental Institute; the Multi-Discipline Engineering Institute at Notre Dame in Indiana; the Energy Efficiency Project at Valparaiso University in Indiana; the Mental Illness and Neuroscience Discovery Institute in New Mexico; Military Spirit in New Mexico; the Academic Center Sustainable Design Project at St. Francis College, New York; the University of Louisville Pediatric Clinical Proteomic Center; the University of Louisville Institute for Advanced Materials; the Advanced Bioreactor located in Butte, Montana; to expand the Center for Integrated and Applied Environmental Toxicology at the University of Southern Maine; the University of Tennessee Cancer Institute; St. Jude Children's Research Hospital in Tennessee; the Huntsman Cancer Institute; the Mega-Voltage Cargo Imaging Development Applications for the Nevada Test Site; the California Hospital Medical Center PET /CT Fusion Imaging System; the Luci Curci Cancer Center Linear Accelerator; Project Intellicare in California; the University Medical Center in Las Vegas, Nevada; the Southern California Water Education Center; Live Cell Molecular Imaging System at the University of Connecticut; the St. Francis Hospital Wilmington, Delaware, MRI and Cardiac Catherization Laboratory; the University of Delaware for the Delaware Biology Institute; the University of Nevada-Las Vegas School of Public Health; the Latino Development and Technology Center; the Swedish American Health Systems; DePaul University Chemistry Lab Renovation Project; the Edward Hospital Cancer Center; the Mary Bird Perkins Cancer Center; the Morgan State University Center for Environmental Toxicology; the Suburban Hospital in Montgomery County, Maryland; the University of Massachusetts at Boston Multidisciplinary Research Facility and Library; the Martha's Vineyard Hospital; the Nevada Cancer Institute; the Mercy Hospital Grayling, Michigan Rural Healthcare Advancement Initiative; the Health Sciences Complex at Creighton University; the Hackensack University Medical Center Women and Children's Pavilion; the Kennedy Health System Linear Accelerator; the University of Buffalo Center of Excellence in Bioinformatics; the Hospital for Special Surgery National Center for Musculoskeletal Research; the New University in New York City; the Radiochemistry research facility at the University of Nevada-Las Vegas; the Hauptman-Woodward Medical Research Institute; the Vermont Institute of Natural Science; and the Tahoe Center for Environmental Services; Southwest Regional Cooling, Heating and Power and Bio-Fuel Application Center; Upgrade Chemistry Laboratories at Drew University, New Jersey; University of Texas Southwestern Medical Center, University of Texas at Dallas Metroplex Comprehensive Imaging Center; Fire Sciences Academy in Elko, Nevada for purposes of capital debt service; and the Desalination plant technology program at UMR.

Congressional direction was provided in FY 2006 for Univ. of Alabama Dept. of Neurobiology to purchase a FMRI; Baylor University Lake Whitney Assessment; SUNY IT Nano-Bio-Molecular Technical Incubator; San Antonio Cancer Center; University of South Alabama Cancer Research Institute; Indiana Wesleyan University Marion for a registered nursing program; Virginia Commonwealth University Massey Cancer Center; Construction of new science facility at Bethel College; University of Wyoming Coalbed Methane research center; Hampton University Cancer Treatment Center; George Mason University research against Biological Agents; Lehigh University

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

Critical Infrastructure Lab.; St. Thomas University Minority Science center; Seton Hall Science/Tech Center; Alvernia College for a Science and Health Building; Institute for Advanced Learning Research Dansville; Galileo Magnet High School Danville; Washington & Jefferson science initiative; Science building at Waubonsee Community College; AVETeC data mamt.electronics and comm. NextEdge Tech.Park; Duchenne Muscular Dystrophy research Univ. of Washington School of Med.; Duchenne Muscular Dystrophy research Children's National Medical Ctr.; Ohio State University for Earth University; Northeast Regional Cancer Institute; Centenary College laboratory; Construction of Science Center at Midwestern Univ.; Univ. of Oklahoma Center Applications Single-Walled Nanotubes; University of Connecticut live cell molecular imaging; University of Central Florida for optics tech in X-Ray; North Shore-Long Island Jewish Health System Breast Cancer Research; Michigan Research Institute Life Science Research Center; Univ. of Arizona Environmental and Natural Resources Phase II; Children's Hospital of Illinois; Research Equipment Coe College; Loma Linda University Medical Center; Triology Linear Accelerator at Owensboro Medical Health System; Burpee Museum of Natural History; Rockford Health Council; Henry Mayo Hospital to purchase new equipment; Washington State University Radio Chemistry; Lapeer Regional Medical Center linear accelerator; University of Nebraska at Kearney; Science Media program at Ball State University; Franklin and Marshall life science building; Boulder City Hospital; Grady Health system disaster preparedness center project; Great Lakes Science Center; Cleveland Clinic Brain Mapping; Roswell Park Cancer Center; St. Marys Cancer Center Long Beach; National Polymer Center at the University of Akron; Biological and Environmental Center at Mystic Aquarium; Riverview Medical Center oncology program; Saratoga Hospital Radiation Therapy Center; State University of New York- Delhi; Kern Medical Center to purchase and install MRI machine; Western Michigan University Geosciences Initiative; Environmental System Center at Syracuse University; SUNY-ESF Woody Biomass Project; ORNL Supercomputer Connectivity NextEdge Technology Park; Oliveit Nazarene University Science Lab; Northern Virginia Comm. College training biotechnology workers; Recording for the Blind and Dyslexic; Eckerd College Science Center; Notre Dame Ecological Genomics Research Institute; Inland Water Environmental Institute; St. Francis Science Center; Medical Research and Robotics, University of Southern California; Hampshire College National Center for Science Education; Pioneer Valley Life Science Initiative Univ. of Massachusetts; MidAmerica Nazarene Univ. nursing biological science program; Westminster College Science Center; City College of San Francisco-Health Related Equipment; Science South Development; St. Joseph Science Center; University North Carolina Biomedical Imaging; Augsburg College; Morehouse School of Medicine; Jersey City Medical Center; University of Rochester James P. Wilmot Cancer Center; Bronx Community College Center for Sustainable Energy; Texas A&M Lake Granbury and Bosque River Assessment; Methodist College Environmental Simulation Research; Brooklyn College Microscope and Imaging Center; Warner Robins Air Logistics Center; University of Chicago Comer Children's Hospital; Martha's Vineyard Hospital; Joint environmental stewardship at SUNY New Paltz and Ulster CC; Central Arkansas Radiation Therapy Institute/Mountain Home; Children's Hospital of Los Angles; Wake Forest University Institute for Regenerative Medicine; Indianapolis Energy Conversion Institute; Philadelphia Educational Advancement Alliance; Barry University-Miami Shores; Montgomery College Biotechnology Project; Purdue Calument Water Institute; University of Chicago Integrated Bioengineering Institute; Mind Institute in New Mexico; Mississippi State University Bio-fuel Application; University of Louisville Institute for Advanced Materials; Center for River Dynamics

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |

and Restoration at Utah State University; Texas Metroplex Comprehensive Imaging Center; Ultra Dense Memory Storage for Supercomputing in Colorado; Health Sciences Research and Education Facility; National Center for Regenerative Medicine; U. of Alabama at Birmingham-Radiation Oncology Functional Imaging Program; University City Science Park, Philadelphia; Jackson State University Bioengineering Complex; Regis University Science Building Renovation Project; St. Jude's Children's Research Hospital; California Hospital Medical Center PET/CT Fusion Imaging System; Mount Sinai Medical Center Imaging and Surgical Equipment; Benedictine University Science Lab & Research Equipment; Swedish American Health Systems; La Rabida Children's Hospital, Chicago; Edward Hospital, Plainfield, IL; Rush Medical Center; Morgan State University Center for Environmental Toxicology; Mt. Sinai Hospital Cardiac Catherization Lab; U. of Mass. at Boston Multi-Disciplinary Research Facility & Library; CIBS Solar Cell Development; University Medical Center of S. Nevada Radiology/Oncology Equip.; Pyramid Lake Paiute Tribe Energy Project; University of Delaware Medical Research Facility; St. Francis Hospital, Delaware Linear Accelerator; Wastewater Pollution and Incinerator Plant in Auburn, NY; South Nassau Hospital Green Building; ViaHealth/Rochester General Hospital Emergency Department; University of Vermont Functional MRI Research; Vermont Institute of Natural Sciences; Castleton State College Math and Science Center; Nevada Cancer Institute; Queen's Medical Center Telemedicine Project; Michigan Technological University Fuel Cell Research; St. Francis Hospital Escanaba, Michigan; Sarcoma Alliance for Research through Collaboration; Hackensack University Medical Center Green Building; Hackensack U. Medical Center Ambulatory Adult Cancer Center; College of New Jersey Genomic Analysis Facility; W. Michigan U. Expanded Energy & Natural Resources Learning Ctr; Arnold Palmer Prostate Center; LA Immersive Tech. Enterprise program at the U. of LA-Lafayette; Brown University MRI Scanner; University of Dubuque Environmental Science Center; New School University in New York City; Oregon Nanoscience and Microbiologies Institute; GeoHeat Center at the Oregon Renewable Energy Center; Portland Center Stage Armory Theater Energy Conservation Project; U. of Massachusetts Medical School NMR Spectrophotometer; Mojave Bird Study; Minnesota Center for Renewable Energy; Science Center at Malby Nature Preserve in Minnesota; Existing Business Enhancement Program Building, U. of N. Iowa; Medical University of South Carolina; Community College of Southern Nevada Transportation Academy; South Dakota State University; Univ. of Arkansas Cancer Research Center; Altair Nanotech; UCLA Institute for Molecular Medicine; New York Structural Biology Center; University of North Dakota Center for Biomass Utilization; St. Joseph College, West Hartford alternative sources of energy dem.project; Portland State University's Solar Photovoltaic Test Facility System; Brockton Photovoltaic Initiative.

| | | | |
|---|---|---|---|
| **Measurement Science** ........................................... | **4,066** | **—** | **—** |

Measurement Science Research is integrated with Medical Applications in FY 2006. There is not a separate request for Measurement Science Research in FY 2007.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| **SBIR/STTR** | **—** | **3,987** | **392** |

In FY 2005 $3,066,000 and $368,000 were transferred to the SBIR and STTR programs, respectively. FY 2006 and FY 2007 amounts are the estimated requirements for continuation of the programs.

| | | | |
|---|---|---|---|
| **Total, Medical Applications and Measurement Science** | **121,924** | **142,563** | **14,000** |

## Explanation of Funding Changes

| | FY 2007 vs. FY 2006 ($000) |
|---|---|
| **Medical Applications** | |
| ▪ Medical Applications Research is held near FY 2006 levels. | +128 |
| ▪ One-time Congressionally directed projects are completed. | -125,096 |
| **Total, Medical Applications** | **-124,968** |
| ▪ **SBIR/STTR** | |
| SBIR/STTR is decreased with the decreased research funding. | -3,595 |
| **Total Funding Change, Medical Applications and Measurement Science** | **-128,563** |

# Construction

## Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| Construction | | | |
| Project Engineering and Design | 9,920 | — | — |

### Description

Facilities to support Genomics: GTL research under the Biological and Environmental Research (BER) program.

### Benefits

The proposed Genomics: GTL Facility for the Production and Characterization of Proteins and Molecular Tags, would surmount a principal roadblock to whole-system analysis by implementing high-throughput production and characterization of microbial proteins. It also would generate protein-tagging reagents for identifying, tracking, quantifying, controlling, capturing, and imaging individual proteins and molecular machines in living systems.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| ▪ **Project Engineering and Design** | **9,920** | **—** | **—** |

Project Engineering and Design (PED) funding supports the proposed Genomics: GTL Facility for the Production and Characterization of Proteins and Molecular Tags was appropriated in FY 2005.

# Capital Operating Expenses and Construction Summary

## Capital Operating Expenses

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2005 | FY 2006 | FY 2007 |
| General Plant Projects | 6,084 | 6,140 | 6,140 |
| Capital Equipment | 18,821 | 11,016 | 26,121 |
| Total Capital Operating Expenses | 24,905 | 17,156 | 32,261 |

## Construction Projects

(dollars in thousands)

| | Total Estimated Cost (TEC) | Prior Year Appropriations | FY 2005 | FY 2006 | FY 2007 | Unappropriated Balance |
|---|---|---|---|---|---|---|
| PED, 05-SC-004 Production and Characterization of Proteins and Molecular Tags | 9,920 | — | 9,920 | — | — | — |
| Total, Construction | | | 9,920 | — | — | |