IV. Science and Technology Strategic Plan

This chapter provides an overview of our strategic plan for research in science and technology. For specific Laboratory program areas, the chapter presents summary plans that describe strategies for accomplishing each program's objectives, in the context of relevant issues and obstacles to be overcome.

Overall coordination of our planning with that of the Department of Energy takes advantage of key DOE and administration planning documents, including the following:

- The national energy policy of the Bush administration, May 2001, a first step toward a comprehensive, long-term national strategy that uses leading-edge technology to produce an integrated national energy, environmental, and economic policy (URL: www.energy.gov/HQPress/releases01/maypr/energy_policy.htm).
- The annual budget request submitted by DOE to Congress (URL: www.cfo.doe.gov/budget/04budget/index.htm), including budget justifications for the Office of Science (URL: www.cfo.doe.gov / budget / 04budget / content/science/science1.pdf) and other DOE offices that support Argonne research.
- The strategic plans of DOE and its Office of Science, which were being updated in April 2003.

Cooperation among the DOE laboratories, particularly through direct R&D collaborations, is increasingly extensive. This trend toward a more integrated laboratory system is described from an Argonne perspective in the Appendix.

A. R&D Area Strategic Plans

The balance of this chapter presents summaries of strategic plans for each of 20 planning units that span our major mission areas (see the inset box on the next page). These strategic plan summaries are grouped into (1) fundamental science and national research facilities, (2) energy and environmental technologies, and (3) national security. This grouping encompasses DOE's four mission areas. In addition, a concluding summary plan addresses the crosscutting topic of collaborative R&D partnerships.

The planning areas for fundamental science and national research facilities correspond closely to the organization of our scientific divisions. In contrast, our technology programs cut across Laboratory divisions to exploit multidisciplinary capabilities. (See the Argonne organization chart at the end of this volume.)

A number of the R&D area plans that follow include discussions of program-specific initiatives. These discussions complement presentation of Argonne's major Laboratory initiatives in Chapter III.

1. Fundamental Science and National Research Facilities

Our activities in the area of fundamental science and national research facilities are supported predominantly by DOE's Office of Science.

a. Advanced Photon Source

Situation

The Advanced Photon Source (APS) is Argonne's premier user research facility. Its ongoing successful operation is central to continuing our outstanding performance in science and technology. Built and operated for DOE-Basic Energy Sciences (DOE-BES), the APS is delivering on its promise to serve the scientific community and to enhance U.S. productivity in a broad spectrum of scientific and technological areas. Over 4,800 individuals have qualified for badges to use the facility, and in 2002 nearly 2,400 unique users performed work there. International competition in this research area

Argonne's Strategic Plans

1. **Fundamental Science and National Research Facilities**
   a. Advanced Photon Source
   b. Materials Science
   c. Chemical Sciences
   d. Nuclear Physics and the Argonne Tandem-Linac Accelerator System
   e. High-Energy Physics
   f. Mathematics, Computing, and Information Sciences
   g. Intense Pulsed Neutron Source
   h. Biosciences
   i. Environmental Research
   j. Science and Engineering Education and University Programs
2. **Energy and Environmental Technologies**
   a. Advanced Nuclear Technology
   b. Energy and Industrial Technologies
   c. Transportation Technologies
   d. Environmental Treatment Technologies
   e. Energy and Environmental Systems
   f. Biotechnology
3. **National Security**
   a. Nuclear National Security
   b. Infrastructure Assurance and Counterterrorism
   c. Department of Homeland Security
4. **Collaborative R&D Partnerships**

comes primarily from two similar synchrotron radiation centers, the European Synchrotron Radiation Facility in France and SPring-8 in Japan.

The APS began operating in 1996 as a user facility serving the worldwide community of x-ray researchers. Between 1989 and 1996, DOE invested $812 million in construction of the APS and in R&D supporting construction. The resulting world-class photon source today provides the brightest x-ray beams available in the United States, for a wide range of research fields such as materials science, structural biology, environmental studies, and applied engineering. Partner users — investigators from private industry, universities, government, and other institutions — have committed, in addition, more that a quarter billion dollars in capital investments for construction of APS beamlines. As of the summer of 2003, 28 of 34 available sectors were assigned to partner users who had formed collaborative access teams (CATs). (A sector comprises one bending magnet beamline and one insertion device beamline.) Included in these 28 sectors are 7 sectors fully operated by Argonne staff, including 1 by the Structural Biology Center (SBC) CAT and 6 by the X-ray Operations and Research section of the APS.

The SBC CAT, a national user facility for the study of macromolecular crystallography, is operated by Argonne's Biosciences Division and funded by DOE's Office of Biological and Environmental Research. Designed for rapid throughput, SBC CAT enables users to collect data by employing standard crystallographic techniques and multiple-energy anomalous-dispersion phasing techniques.

Two of the six sectors operated by the APS X-ray Operations and Research section began as a joint venture of Argonne's Chemistry and Materials Science Divisions, in partnership with the DOE-BES Geosciences program and Northern Illinois University. Those two sectors have been developed and instrumented for research in materials science, chemical science, atomic physics, solid state physics, and the geosciences.

The other four sectors operated by the APS X-ray Operations and Research section were originally designed and constructed by APS staff. These sectors focus on developing instrumentation and techniques that utilize the unique properties of APS radiation to advance the frontiers of scientific research capabilities. Among the capabilities developed are microbeam techniques, nuclear resonant spectroscopy, high-resolution inelastic x-ray scattering, coherence-based techniques, applications of high-energy x-rays, and the generation and use of polarized x-rays. The microbeam optics developed are providing foundations for the nanoprobe beamline that will be associated with the Center for Nanoscale Materials (CNM; see Section III.A.1), and the inelastic scattering program spawned the development of an entire APS sector devoted to inelastic x-ray scattering.

In addition to these six sectors, APS jointly operates three other sectors (in partnership with their respective CATs), providing funding and staff for operations and user support.

Demand is high for the remaining six unassigned APS sectors. One sector has been requested for structural biology research, and four other sectors have been requested for materials science (including the sectors for inelastic scattering and the nanoprobe beamline) and for environmental science. Decisions regarding assignment of the remaining sectors will be made over the next several years.

The APS provides 5,000 hours of user beam time each year. During 2002 the APS provided users with top-up (constant-current) beams — an operational mode pioneered at the APS and now used at other facilities — during 75% of their scheduled beam time. This achievement increases the number of ampere-hours delivered; facilitates beam stability because of the constancy of the power loading on the storage ring and optical components; and permits ring operation at lower emittance, because beam lifetime is no longer a concern. In 2002 the availability of APS beam time (the percentage of scheduled user beam time actually delivered) reached a new high of more than 97%.

Vision

The APS will continue to operate at current high reliability levels and will remain the preeminent source of hard x-rays for the U.S. research community into the foreseeable future. The facility will serve a wide range of frontier science and technology and will support investigations of importance to both science and national security. To maintain the high reliability of the accelerator and beamlines, we will implement innovative accelerator enhancements that further improve beam characteristics, as well as state-of-the-art technology that improves experimental capabilities. Through productive partnerships we will serve APS users better, thereby creating a rewarding and enriching R&D environment and enhancing the facility's worldwide leadership role.

Mission, Goals, and Objectives

The mission of the APS is to deliver world-class science and technology by operating an outstanding synchrotron radiation research facility accessible to a broad spectrum of researchers.

Overall goals are as follows:

- Operate a highly reliable third-generation source of synchrotron x-ray radiation.
- Foster a productive environment for conducting research.
- Enhance the capabilities available to facility users.
- Assure the safety of facility users and staff, as well as protection of the environment.
- Maintain an organization that provides a rewarding environment fostering professional growth.
- Optimize scientific and technological contributions to DOE and society from research carried out at the APS.

Major objectives for FY 2004 are as follows:

- Maintain the availability of accelerator operations at better than 95%.
- Maintain operating time scheduled for users at 5,000 hours.
- Provide APS users with essential services in the areas of technical support, operations, safety, administration, and general services.

Issues and Strategies

A major challenge for the APS is providing operational support for sectors originally constructed with funding from DOE-BES. To aid in the implementation of this new operational mode, we have developed a new, more flexible model for partnering with APS users. "Partner users" include members of the previous CATs and may also include groups involved in focused projects of smaller scope that make lasting improvements to the facility. (Other users are "general users.") We will continue to evaluate this new user model. In any case, optimizing the scientific productivity of these beamlines will require additional annual resources averaging $1.5 million per sector.

To date, all sectors assigned to partner users have an associated laboratory-office module for operational staff. Five additional prospective partner user groups are in various stages of writing proposals and raising funds, and the majority of those groups are expected to be approved within the next few years. Two are associated with facilities proposed as part of major Laboratory initiatives. First, the nanoprobe beamline will be associated with the CNM (see Section III.A.1); it will provide the capabilities needed to characterize and study nanostructures though a variety of techniques. Second, an additional sector is proposed as a high-throughput macromolecular crystallography beamline associated with Argonne's Functional Genomics initiative (see Section III.A.3). This beamline will focus on biostructures as they relate to structural genomics. Buildings for these proposed centers will be near the APS and will provide laboratory and office support for associated beamline users. However, no laboratory-office module currently exists to support the remaining prospective groups. Funding for the final laboratory-office module is required now so that the building will be available when it is needed for the proposed beamlines. Additional funding will also be needed to upgrade building services (e.g., heating and cooling).

The APS is a high-quality research facility with excellent, experienced staff. Although all of the technical design parameters of its accelerator systems have been achieved, the facility's staff continue to focus on responding to ever-increasing user demands for the best possible operational reliability and availability. To remain at the scientific forefront and maintain the excellence of its in-house research staff, the APS must continue to develop and meet technically challenging research objectives in accelerator physics, insertion device development, beamline design, optics R&D, and other areas.

Initiative: Enhancement of the APS and Development of Future Light Sources

Over the past three decades, the brilliance of x-ray sources has doubled every ten months. Use of coherent flux, which is directly proportional to beam brilliance, has had major unforeseen benefits for work in the life sciences, research on soft condensed matter, and materials science, even though the flux values currently available at the APS are relatively low. To achieve the benefits expected from future experiments at higher brilliance, planning must begin now for a 10- to 100-fold increase in APS beam brilliance.

Over the next 20 years, new and exciting x-ray sources based on energy recovery linacs (ERLs) and free-electron lasers (FELs) will be needed in the United States. These sources are not simple enhancements of third-generation sources. Rather, they are a new breed of sources having new properties and applications. Although some users of today's synchrotron radiation sources may become users of these new facilities, ERLs and FELs will not replace existing sources for most of today's researchers. Therefore, the APS must remain at the cutting edge of third-generation synchrotron radiation technology, where the demand for x-rays will not decrease for the next 20 years or more. At the request of DOE, we recently developed a 20-year upgrade plan for the APS that is organized into four temporally overlapping phases:

- *Phase I*. Complete beamline installations on the remainder of the storage ring and maximize operations at existing beamlines. This phase, which has already begun, is expected to extend over the next eight years.
- *Phase II*. Optimize source characteristics. This phase will overlap Phase I, beginning during FY 2004-FY 2005 and continuing for approximately a decade.
- *Phase III*. Develop the next-generation user facility by improving the efficiency and performance of beamlines and taking advantage of advanced detectors, robotics, and automation. This phase will start in full in approximately eight to ten years.
- *Phase IV*. Implement a major upgrade of the accelerator complex to develop a "super storage ring." Work on this final phase will begin about ten years from now and will last for approximately ten years. To minimize disruption to APS beam time, for which demand will continue, plans call for only one extended shutdown of the APS — for

implementation of a new linac and storage ring.

Phase I. The clearly appropriate focus of the first phase of a 20-year plan for the APS is full use of the storage ring. We expect that construction of about ten new beamlines will begin during FY 2004-FY 2012, taking advantage of the four remaining unassigned sectors (with two beamlines per sector) and the installation of several bending magnet beamlines. These ten new beamlines do not include (1) three sectors dedicated to macromolecular crystallography, where construction is about to begin (funded by non-DOE sources) and (2) the insertion device beamlines for two exciting proposals whose construction has been partially funded by DOE-BES — the inelastic x-ray scattering beamline and the nanoprobe beamline to be associated with the CNM. The average time from conception of a beamline to commissioning and start of user operations is approximately five years, so construction at the remaining available APS sectors is expected to continue through the next decade.

In parallel with construction of new beamlines, we must contend with the aging of existing beamlines. Ten years have passed since the original design of several beamlines. They will need major refurbishments over the next decade to take advantage of recent major advances in optics and instrumentation. Many beamlines can no longer meet the ever-increasing technical requirements of their users, or they simply fall short of optimal performance levels. This problem is compounded because storage ring operating parameters today are much better than the original specifications on which beamline designs were based. Development of state-of-the-art detectors is perhaps most urgent. In many cases, better detectors are already on the critical path to achieving faster data collection. Construction and refurbishment of some aging beamlines will be the responsibility of the APS, either alone or in collaboration with partner users. The proposed science to be performed at those beamlines will drive the new construction and upgrades. The APS will rely heavily on guidance from its Scientific Advisory Committee in determining which beamlines will be built and upgraded.

Future beamlines are expected to fall into two major categories: (1) those used for “routine data collection,” which need to be provided as “turn-key” facilities, and (2) cutting-edge beamlines optimized for “experiments,” where constant innovation and tweaking are necessary for scientific success. The highly specialized beamlines in the second category are being designed for radiation properties optimized to particular types of research, such as inelastic x-ray scattering, high-energy x-ray scattering, or nanoprobe applications. Therefore, concurrent with development of new beamlines under Phase I, the aggressive source development specified in Phase II is also needed.

Phase II. Given limitations imposed by the current magnetic lattice of the APS storage ring, further reductions in the natural emittance (presently better than the original design specification by a factor of almost three) can be only incremental. Therefore, without major reconstruction of the storage ring, significant increases in beam brilliance must come through the development of optimized insertion devices or increases in circulating beam current. Along with new insertion devices and higher current, compatible front ends and optical components will also be required. Replacement or upgrading of all original front ends will probably be needed to meet the thermal requirements of longer insertion devices and higher currents. The combination of optimized insertion devices, improved optics, and higher beam currents could improve effective brilliance by more than an order of magnitude.

Insertion device development will push toward shorter-period devices capable of higher energies (20-45 keV) with the first harmonic. We believe that the most promising approach to this development involves use of superconducting undulators. Increased brilliance at high photon energies (25 keV and above) will improve inelastic x-ray scattering capabilities and provide an unequaled source of high-brilliance hard x-rays for high-energy elastic scattering.

To improve beam brilliance further, we have begun to explore the possibility of increasing the length of straight sections in the storage ring to accommodate longer or multiple insertion devices. Initial results indicate that modifications of the storage ring lattice in a few places around the ring could increase the clear space for insertion devices to ten meters from the present five meters. Increased brilliance will be particularly important for certain cutting-edge, photon-hungry experiments, such as inelastic scattering, high-resolution imaging, correlation spectroscopy, and time-resolved studies. Longer straight sections would also allow installation of elliptically polarizing undulators optimized from 0.5 to 3 keV. The beam brilliance from these devices would result in a world-class beamline for photoemission and a photoemission electron microscope capable of spatial resolutions of a few nanometers, well suited to studying the magnetic properties of materials. Despite the common idea that high-energy storage rings are associated with the production of hard x-rays, 6-8 GeV is in fact an ideal stored-beam energy for generating elliptically polarized soft x-rays. This fact, combined with the inherently superior stability of higher-energy beams, means that high-energy storage rings have considerable advantage in generating high-quality polarized soft x-ray beams. The APS is likely to remain the only high-energy third-generation storage ring in the United States for the foreseeable future.

In addition to superconducting and polarizing undulators, Phase II will also pursue solenoid-driven undulators. Insertion devices based on solenoids can simultaneously have both variable periods and variable fields (in contrast to present-day devices having fixed periods and variable fields), making them valuable for a host of scientific applications requiring optimization in several different energy ranges.

As noted above, substantial reduction in the natural emittance of the APS is unlikely with its present lattice. However, the effective emittance delivered to users can be improved by enhancing beam stability. Phase II will therefore continue the focus on this effort. Phase II will also focus on reducing the size and duration of perturbations of the stored beam during the top-up process, which will further enhance beam quality.

Phases III and IV. To adequately accommodate the estimated 10,000 researchers who will use the APS during the coming decade, Phase III will improve ease of access, beamline performance, and data collection speed. Automation and robotics for sample alignment have already been implemented on macromolecular crystallography beamlines at the APS and elsewhere. Many physical science beamlines could benefit from implementation of similar techniques. For instance, integration of automated sample changers into powder diffraction beamlines and small-angle-scattering beamlines seems to be a straightforward extension of the sample changers used for macromolecular crystallography. Moreover, automated alignment of optical components and diffractometers could substantially increase scientific productivity of some beamlines (particularly the turn-key beamlines proposed for Phase I); automation should be incorporated into the design of these beamlines from the beginning. We also see a large class of experiments that could be performed effectively via remote access, if we can achieve real-time communication of data, experimental conditions, and beamline control.

Phase IV envisions significant improvements in the accelerator system. As indicated above, maintaining the existing 40-fold symmetry of the storage ring implies that only incremental improvements in particle beam brilliance can be expected. Phase IV calls for a radical change in the storage ring magnetic lattice, from 40-fold symmetry to 80-fold, that will reduce beam emittance by a factor of eight. This eightfold increase in beam brilliance — in combination with the increased brilliance achieved through optimized insertion devices, longer straight sections, and increased current — would put the APS near the limit of brilliance attainable with a storage ring of its dimensions and energy. The resulting super storage ring would significantly benefit the many important brilliance-related techniques, notably x-ray photon correlation spectroscopy, coherent imaging, inelastic scattering, and x-ray nanoprobe microscopes. The obvious advantage of the Phase IV approach to a super storage ring is its continued use of existing beamlines. The novel concepts proposed would create new capabilities that are qualitatively and quantitatively different, and considerable R&D will be required to verify the feasibility of the proposed alterations of the storage ring. Modification of the APS storage ring for reduced emittance would not be implemented until very late in the 20-year plan.

Required resources for the first eight years of the APS upgrade plan are summarized in Table IV.1. Funding will be sought from DOE-BES (KC).

Table IV.1 Enhancement of the APS and Development of Future Light Sources
($ in millions BA, personnel in FTE)

	FY05	FY06	FY07	FY08	FY09	FY10	FY11	FY12
Costs								
Operating	3.6	5.6	8.0	8.2	9.0	7.5	7.5	7.5
Capital Equipment	16.4	19.4	22.0	24.3	23.5	20.0	20.0	20.0
Construction	-	-	-	-	-	-	-	-
Total	20.0	25.0	30.0	32.5	32.5	27.5	27.5	27.5
Direct Personnel	14.0	23.0	35.0	35.0	39.0	32.0	32.0	32.0

Initiative: Generation and Use of Short-Pulse Radiation from Free-Electron Lasers

In the late 1990s the Basic Energy Sciences Advisory Committee (BESAC) gave first priority to R&D on sources exploiting an 8- to 20-keV x-ray laser. We have joined five partners — Brookhaven, Los Alamos, and Lawrence Livermore National Laboratories; the Stanford Linear Accelerator Center (SLAC); and the University of California at Los Angeles — to develop a proposal for a laser in the required wavelength range. Development of the proposed facility, the Linac Coherent Light Source (LCLS), will make use of the two-mile linear accelerator at SLAC and will take advantage of the distinctive capabilities of each of the partner institutions. We have agreed to develop the integrated undulator systems for the LCLS, which will account for about 20% of the total estimated project cost. This work will be funded separately from APS operations.

The original LCLS Scientific Advisory Committee, led by Gopal Shenoy (Argonne) and Joachim Stohr (Stanford University), gave BESAC a detailed proposal for pioneering experiments in atomic, molecular, plasma, and laser physics; in protein crystallography; and in nanoscale dynamics in condensed matter. Argonne researchers must start now to develop the optics, instrumentation, beamlines, and experimental techniques for the next generation of laser-based x-ray experiments, if they are to lead the use of the LCLS and remain at the forefront of synchrotron radiation research. For example, this unique facility will undoubtedly have major scientific impact in areas such as femtosecond time-resolved studies. The expertise needed for such studies should be developed now, so high priority should be given to a strong program of pump-probe studies using the APS with its current characteristics. Time-resolved studies, currently under way at the APS though in a nascent stage, should be expanded in scope and enhanced to improve temporal resolution, in order to exploit fully the unique science achievable through this largely unexplored field of study. To gain valuable experience in the use of femtosecond x-ray pulses, we are actively participating in the Sub-Picosecond Photon Source project being developed at SLAC, which aims to produce femtosecond electron pulses at the existing two-mile linac. The APS is providing the required insertion device, and APS staff are involved in experimental investigations of uses for those x-rays. First light from the project was obtained in the summer of 2003.

To further explore the physics and scientific applications of short-pulse radiation from FELs, we are developing a proposal for a partner user program to enhance operation and use of the vacuum ultraviolet FEL at the APS. Unlike users of other synchrotron-based facilities, FEL user partners would not use x-rays from a storage ring source. Rather, they would use ultraviolet radiation generated by an FEL on the low-energy undulator test line at the APS. No tunable laser systems existing today can access the wavelength range below roughly 150 nanometers. This very interesting wavelength range is still virtually unexplored by any tunable, high-power femtosecond laser system anywhere in the world.

Required resources are described in Table IV.2. Funding will be sought from DOE-BES (KC).

Table IV.2 Generation and Use of Short-Pulse Radiation from Free-Electron Lasers
($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	-	-	1.8	2.0	1.1	-	-
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	-	-	1.8	2.0	1.1	-	-
Direct Personnel	-	-	4.3	3.8	0.8	-	-

b. Materials Science

Situation

Our research in materials science addresses critical issues underlying the development of new and improved materials that play crucial roles in both the national economy and DOE mission areas. Our work embraces experimental and theoretical studies, as well as computer simulations. Laboratory programs provide the fundamental understanding of novel materials that will underpin tomorrow's technologies. These programs emphasize the broad scale and depth of investigation that are possible within the national laboratories.

Our user facilities for materials research feature prominently in Laboratory research programs. We play a leading role in developing the instrumentation and experimental design needed to apply our facilities to problems at the frontiers of materials science. Our programs stress collaborations with leading scientists at the Laboratory, across the nation, and around the world.

Key materials research areas at Argonne include superconductivity, magnetism, ferroelectricity, ceramic films, metals, carbon, biomaterials, and nanoscale materials science and technology. Crosscutting research themes are emphasized, especially complex oxides, interfaces, and defect production.

Vision

We will foster world-class materials science, forefront instrumentation, and unique user facilities. The combination of individual freedom and teamwork that nurtured past successes will be strengthened. Our contributions to new materials, especially at the nanoscale, will support both DOE and the nation in meeting new scientific, technological, and economic goals.

Objectives

Specific objectives of our research are as follows:

- Develop forefront programs in nanoscale materials science that explore the effects of confinement, proximity, and organization in magnets, superconductors, and ferroelectrics.
- Develop innovative neutron scattering science and apply it to the investigation of materials, in preparation for the advent of the Spallation Neutron Source.
- Understand and exploit the rich diversity of behavior in complex materials, including oxides, polymers, biosynthetic composites, and carbon.
- Develop novel instrumentation that drives the frontier of science at the APS and the Electron Microscopy Center (EMC).

Issues and Strategies

Today is a time of high opportunity in condensed matter and materials physics. National attention on nanoscience has revealed new horizons for creating, understanding, and controlling novel behavior in materials arising from their nanoscale structure. Now within reach are grand challenges in materials fabrication by lithography and self-assembly, as well as in materials characterization using scanning probe microscopy, electron microscopy, focused x-ray scattering, and neutron scattering. Moreover, a complementary national emphasis on biology and medicine reveals many opportunities for adapting the traditional tools and ideas of materials physics to the study of genomes, proteins, and living cells. Qualitatively new materials and functionality can be created at the "hard-soft" interface between biology and condensed matter. All these directions are part of a general trend in materials physics toward increasing complexity. Exploiting this rich diversity of behavior will require new concepts and new approaches to integrating interdisciplinary experiments and theory in a comprehensive research program.

We will take advantage of these unusual opportunities to strengthen our contributions to materials science. Creation of a new CNM (see Section III.A.1) will extend the Laboratory's reach in materials science through development of fabrication facilities, a nanoprobe x-ray beamline at the APS, and new nanoscale characterization instruments. With other national laboratories, we are developing a Transmission Electron Aberration-Corrected Microscope that will bring subnanometer spatial resolution and real-time response to a host of new materials experiments. We are launching new programs in biosynthetic materials and spin-electronic materials and are teaming with other national laboratories to develop Centers of Excellence in Synthesis and Processing, in the areas of granular materials, permanent magnetism, ultrananocrystalline diamond, and ferroelectrics.

We emphasize excellent basic science as the cornerstone of our materials science program. We continuously refresh our program mix by adding new directions as new materials are discovered and research capabilities grow. We stress comprehensive programs that incorporate integrated experimental and theoretical thrusts and exploit advanced scientific instrumentation ranging from benchtop scanning probes to unique x-ray and neutron sources. We regularly attract outstanding international scientists as collaborators in our interdisciplinary programs. Leading theorists are attracted to our new Materials Theory Institute for stays of one week to six months in support of key experimental programs. The resulting extensive professional network is invaluable as a source of intellectual stimulation and also as a source of outstanding candidates for postdoctoral and permanent staff positions.

We have launched an interdisciplinary program for the design, synthesis, and characterization of a new class of nanostructured biocomposite materials that exploit the capabilities of biological molecules to store and transduce energy. The goal is to organize complex biological molecules (e.g., light-harvesting proteins) into artificial host structures where the biological function can be optimized and exploited. An interdisciplinary team of materials scientists, chemists, and biologists will use a novel lipid-based complex fluid and a rigid mesoporous inorganic framework as the host materials for biomolecules. This novel approach to nanostructured biomaterials that exploit biological functions has great scientific interest and enormous technological value. Research results are expected to provide fundamental insight into ways to use soft and hard materials to construct complex architectures that combine the functionality of biomolecules with the novel properties of host materials. This work will also provide fundamental knowledge of (1) nanoscale phenomena occurring at the interfaces between the integrated materials and (2) means to tailor energy transduction processes. Results could lay the groundwork for producing the next generation of materials for use in sensors, optoelectronics, artificial organs, and catalysis. This program will use major Argonne research facilities, including the APS, the EMC, the Intense Pulsed Neutron Source (IPNS), the Advanced Computer Research Facility, and the new CNM (see Section III.A.1). Also available for this work will be the facilities of the Center for Nanofabrication and Molecular Self-Assembly at Northwestern University. These major facilities provide unique capabilities for synthesizing and characterizing new biomaterials, as well as for understanding and tailoring their properties. This program was funded at the end of FY 2002 by DOE-BES through its program Nanoscale Science, Engineering, and Technology Research.

User Facility: Electron Microscopy Center

Situation

Argonne's EMC provides transmission and scanning electron microscopy for high-spatial-resolution imaging, microanalysis, and *in situ* research. The EMC includes the Intermediate Voltage Electron Microscope (IVEM)-Tandem, which is employed for a variety of *in situ* studies, especially for dynamic recording and structural characterization of the effects of ion irradiation. The IVEM-Tandem is the only facility in the Americas with this specialized capability, and it is used by the international community. Qualified users access the IVEM-Tandem by submitting written proposals that are peer reviewed. For nonproprietary research there are no use charges. EMC users — including researchers from universities, other national laboratories, and industry — conduct studies ranging from imaging of electron-sensitive soft materials to *in situ* observations of phenomena at elevated and cryogenic temperatures in pure metals and alloys, semiconductors, and ceramics.

Other advanced instrumentation in the EMC includes a state-of-the-art transmission electron microscope (TEM) with a field emission gun, excellent analytical capabilities, and the capability to perform holographic and Lorentz imaging. A high-resolution scanning electron microscope (SEM) with a field emission source provides a broad range of capabilities in surface analysis. We are in the process of acquiring new instrumentation using focused-ion-beam techniques for manipulating and modifying samples on the nanoscale. The EMC continues to drive important developments in its field. We are currently pursuing an aberration-corrected TEM that will provide unprecedented capabilities for *in situ* experiments and will be ideally suited to comprehensive diffraction and spectroscopy studies of single nanoparticles in controlled magnetic environments.

Vision

The EMC will develop new techniques and methods and state-of-the-art TEM and SEM instrumentation, including capabilities for *in situ* studies. The materials research supported will provide important new insights for major technologies in such areas as micromagnetics, irradiation effects in high-temperature superconductors, solid-state amorphization reactions, and analysis and control of nanostructures.

Issues and Strategies

Our IVEM-Tandem facility provides ion beam capability for *in situ* studies and in this role remains a special resource for the national research community. The EMC is developing a new program to improve *in situ* experimentation based on novel designs for holders and samples. These advances will serve as an important foundation for a major new initiative in aberration correction for electron microscopy. At the same time, the EMC will develop new methods and capabilities for imaging and diffraction of single nanoparticles, especially position-sensitive diffraction.

A major issue in the current EMC experimental space is high levels of vibrational, electromagnetic, and thermal noise that reduce the effectiveness of the facility's electron microscopes. The most advanced microscopes cannot operate at their designed specifications because of the mechanical vibration of the floor. Vibration and other noise problems are inherent in a building constructed in the mid 1960s and designed for other uses. Required noise isolation will become much more stringent for the aberration-corrected microscopes to be developed under the initiative described below. This level of noise isolation can be achieved only in a new, state-of-the-art building designed to have quiet floors, electromagnetically shielded rooms, and precise temperature control. Ideally, such a dedicated noise-free building would be located near complementary facilities such as the Center for Nanoscale Materials. Experimental samples fabricated in the Center for Nanoscale Materials could then be characterized conveniently by using the electron microscopy.

Initiative: National Transmission Electron Achromatic Microscope

Thanks to advances in aberration correction and quantitative-transmission electron microscopy, a new generation of electron microscopes can be built that are capable of sub-angstrom image resolution and sub-electron-volt spectroscopic resolution and that have space adequate for a variety of important experiments on advanced materials. To take advantage of these new technologies, the EMC is participating in the proposed Transmission Electron Aberration-Corrected Microscope (TEAM) project. The required instrument development will be carried out cooperatively at DOE's four national centers for electron beam microcharacterization, with each center contributing a complementary specialized facility based on a common platform.

The revolutionary combination of space and resolution envisioned for TEAM instruments will allow the electron microscope to be converted into a true experimental materials science laboratory. Scientific benefits to be expected include the first three-dimensional atomic imaging of defect structures; the first atomic structure determination of a glass; microscopic understanding of magnetism and ferroelectricity in nanostructures; visualization of dislocation interactions in nanostructures under controlled stress; development of interface science to the level of surface science; understanding of grain boundary motion under stress in nanocrystals; understanding of chemical reactions on highly curved, small catalyst particles; and imaging of defects in the oxygen sublattice of complex oxides. More generally, advances in electron beam micro-characterization associated with the development of TEAM will be crucial for proper implementation of the planned national thrust in nanotechnology. The TEAM project will also help to revitalize the critically important electron optics industry in the United States.

Following an international workshop held at Argonne in FY 2000 and a second workshop held at Berkeley Lab in FY 2002, the EMC is receiving preliminary funding to develop the new electron-optic designs necessary to incorporate aberration correction in electron microscopes. This work will include a broader program in aberration correction for charged-particle optics. The focus will be a novel design that enables excellent control of the magnetic environment around the sample, a requisite for studying magnetism at the atomic scale. These efforts will contribute importantly to Argonne's growing research in nanoscience.

Funding will be sought from the DOE-BES Materials Science program (KC-02). Partnerships with industry and universities that have already been developed will be an important component of this new Argonne initiative.

c. Chemical Sciences

Situation

Chemistry is an Argonne core capability. World-class research programs and staff with cutting-edge expertise study fundamental scientific questions critical to DOE's mission. Our research provides the foundations for addressing issues of energy independence, environmental sustainability, and national security, and it will underpin new technologies for energy efficiency, energy conversion, combustion, nanotechnology, cleanup and disposal of radioactive and nonradioactive waste, and catalysis.

Vision

We will enhance our status as a leading performer in chemical science research by sustaining our preeminence in established research focus areas, by seeking new initiatives, and by forging new collaborations based on our core competencies to pursue new multidisciplinary research challenges.

Objectives

Our chemical science program will grow around our core competencies — in physical chemistry, chemical dynamics, and chemical energy sciences — to focus aggressively on important new research areas by developing closer ties within the chemical sciences program and with other programs at Argonne and the University of Chicago. Our objective is to foster cross-disciplinary collaborations that will provide revolutionary approaches to difficult problems in chemical science. Major long-range objectives of Argonne's core research in the chemical sciences are as follows:

- Investigate issues related to interfacial dynamics and to gas- and condensed-phase chemistry, in order to broaden our expertise both in experimentation and in theory and computation, with the goal of understanding chemical reactivity in all forms.
- Examine the chemical and physical properties of nanoscale materials — including gas-phase clusters, colloids in solution, hybrid bioinorganic systems, and nanomaterial on or in bulk phases — through studies combining experimentation and theory.
- Improve understanding of the fundamental fast-transient physicochemical phenomena that occur when radiation interacts with matter, in the context of
  - Photochemical energy conversion in natural photosynthetic systems and comparisons with photochemistry in synthetic systems,
  - Charge dynamics and transport in the condensed phase, and
  - Gas-phase photoionization and x-ray interactions with atoms and molecules.
- Develop expertise and facilities to investigate the fundamental chemical and physical properties of actinides.

Essential to achieving these objectives are the development and use of special tools and facilities, including the following:

- Specialized capabilities at the APS, including transient x-ray spectroscopies (x-ray absorption and scattering); hard x-ray physics (atomic, molecular, and optical); and the Actinide Facility for experiments involving samples that contain such elements
- Novel electron and x-ray generators
- Time-domain, multifrequency capabilities for electron paramagnetic resonance
- Transient optical spectroscopies
- Scalable software for theoretical chemistry simulations, optimized to run on large centralized parallel computer platforms at Argonne and elsewhere

Issues and Strategies

Our core chemical sciences research programs integrate special expertise with unique tools and facilities. The recent developments described below are establishing new directions in chemical sciences research that are consistent with DOE's energy mission. In addition to support from DOE-BES, we will explore a broad range of further funding sources for studies in these new directions.

In this context, important recent developments include the following:

- We are investigating new ideas about hydrogen production and storage on the basis of our recent discoveries in such diverse areas as synthesis of template-derived carbon nanofibers, the reduction power of irradiated metal oxide colloids, and bonding patterns in organic-inorganic hybrids. (See the major Laboratory initiative Hydrogen Research and Development in Section III.B.2.)
- Our developing capabilities for synthesizing nanoparticles can address fundamental questions about reactivity and promise novel approaches to organized assembly. We are also developing tools to study electronic structure in confined spaces; to observe the migration of charge, photons, and spin; and to understand the high efficiency and selectivity of catalysis on the molecular scale.
- We are gaining valuable experience in areas of research at the inorganic-biochemical interface; state-of-the-art time-resolved x-ray capabilities on molecular and kinetic time scales; completion of the first phase of the tabletop terawatt laser for ultrafast pulse radiolysis; and rapidly expanding computational chemistry power on local and remote parallel facilities. The resulting synergistic capabilities are providing critical mass to address issues in complexity and in collective phenomena, including particle aggregation and disaggregation in inorganic systems and protein dynamics in biological systems.

The chemical science goals in the major Laboratory initiative Center for Nanoscale Materials (Section III.A.1) derive directly from Argonne's core expertise in areas including (1) the assembly of nanostructures from gas-phase clusters or fluidic phases, focusing on understanding the forces that drive aggregation and developing experimental and theoretical methods for controlling the assembly of nanostructures; (2) controlled reactivity in hybrid nanostructures, focusing on understanding and controlling photochemical, catalytic, and biological reactivity in bioinorganic hybrids and mesoporous structures at the nanoscale (an area in which the project Nano-Engineering the Biomolecule-Inorganic Interface for Integrated Photochemistry and Catalysis has been funded); and (3) information transfer between nanodomains, focusing on understanding the principles by which the communication between nanoscale devices (sending and receiving) can be organized and controlled. Our expertise in transient spectroscopies, x-ray synchrotron science, photochemistry, and theory, coupled with emerging expertise in scanning-probe microscopy, will be critical for understanding these phenomena. We have initiated a program in nanophotonics for these studies.

Our integrated program in the fundamental chemistry of radioactive waste is partly supported by the DOE Environmental Management Science Program. We are uniquely qualified to undertake this program through our core capabilities in chemical separations science, heavy-element chemistry, radiation chemistry, and theoretical chemistry, as well as through our facilities for research with radioactive materials (including the Actinide Facility at the APS and our nuclear magnetic resonance (NMR) facility designed for studying radioactive materials). This program of experimental and theoretical research responds to a national need for greater fundamental knowledge of the chemistry underpinning technologies for the cleanup and disposal of radioactive waste.

We have developed two research programs in the chemical sciences in response to DOE's Nuclear Energy Research Initiative (NERI). Both were awarded funding in 2002. One program focuses on (1) an innovative, single-material, minimum-volume approach to the selective sorption of most metal ion radionuclides from aqueous waste solutions and (2) the subsequent creation of a final nuclear waste form that is suitable for long-term storage or burial. In the other NERI research program, we are collaborating with the University of Wisconsin to study radiation-induced corrosion relevant to designing next-generation reactors. Higher energy efficiency can be achieved by operating pressurized-water reactors at pressures and temperatures well beyond those necessary for the formation of supercritical water. This work will consider the possibility of radiolytic water decomposition under such conditions.

We are partnering with Northwestern University in the Institute for Environmental Catalysis. This partnership takes advantage of our expertise in magnetic resonance, pulse radiolysis, synchrotron research at the APS, and heterogeneous catalysis. In a second institute, we are a partner with Ohio State University in research on the role of environmental molecular interfaces in the chemical and biological reactivity of pollutants. This collaboration will leverage our expertise in solid-state NMR, high-field electron paramagnetic resonance, and surface science. In a third partnership, we have joined the University of Notre Dame in studies on actinide chemistry that exploit our facilities and expertise in radionuclide chemistry.

We have developed a new program in computational chemistry in response to DOE's Scientific Discovery through Advanced Computing initiative. Conducted in collaboration with Sandia National Laboratories and several universities, the program focuses on software for calculating and applying reaction kinetics and dynamics. This effort exploits our expertise in chemical dynamics, theoretical chemistry, and computer science and is part of the multi-laboratory initiative Chemical Science Discovery through Advanced Computing: A Multi-Scale Collaboration. A second part of this program will develop the foundation for statistical methods and algorithms that provide internally consistent tables of active thermodynamic values.

d. Nuclear Physics and the Argonne Tandem-Linac Accelerator System

Situation

Review committees have consistently identified Argonne as one of the world's centers of excellence in nuclear physics research. Our leadership role in planning the Rare Isotope Accelerator, the next-generation nuclear physics accelerator, will continue this tradition. The Argonne program has many strengths, including (1) low-energy heavy-ion physics, which is largely performed at the Argonne Tandem-Linac Accelerator System (ATLAS) facility (discussed below); (2) medium-energy nuclear physics, which emphasizes the use of lepton beams (at Fermilab, TJNAF [the Thomas Jefferson National Accelerator Facility], and DESY [Deutsche Elektronen Synchrotron]) as probes into the nuclear medium; (3) the study of relativistic heavy-ion collision dynamics by using beams from Brookhaven's newly commissioned RHIC (Relativistic Heavy Ion Collider); and (4) nuclear theory, which focuses on developing fundamental understanding of hadronic and nuclear structure, reactions, and dynamics.

Vision

Our nuclear physics program will resolve fundamental questions concerning the characteristics and dynamics of nuclear and subnuclear degrees of freedom in nuclei and nuclear matter. This work will involve continuous development of more powerful research apparatus and methods and the use of unique research facilities at Argonne and throughout the world.

Objectives, Issues, and Strategies

Our work in low-energy heavy-ion physics will take full advantage of the unique capabilities of ATLAS to explore and understand nuclei at the limits of their stability: at high excitation energies, in exotic shapes, at rapid rotation, and with extreme proton-to-neutron ratios. Producing and detecting previously unknown isotopes and studying their structures can benefit greatly from secondary (radioactive) beams, which can provide access to regions of nuclei not currently accessible with stable beams. This approach will also allow laboratory study of key reactions in astrophysics and in the creation of the elements — reactions that occur in astrophysical settings and involve short-lived nuclei. To this end, we are proposing a national Rare Isotope Accelerator that will be based largely on novel superconducting accelerator technology originally developed at the Laboratory and used for ATLAS. (See Section III.A.2.)

Our work in medium-energy nuclear physics uses energetic lepton beams to increase understanding of quark and meson degrees of freedom in nuclei and the role of the quark-gluon structure of nucleons in shaping the character of nuclear forces. Argonne researchers are playing a leading role in the research program at TJNAF, emphasizing the use of a general-purpose magnetic spectrometer we constructed at the facility. At DESY the Argonne group emphasizes use of a dual-radiator ring-imaging Cerenkov detector in the Hermes experiment to study the spin structure of the proton. In addition, we are developing new technologies in laser atom trapping of noble gas atoms for sensitive trace isotope analyses and for tests of fundamental symmetries.

Our work in nuclear theory addresses the dynamics, structure, and reactions of (1) quark and gluon degrees of freedom in hadrons and (2) meson, nucleon, and nucleon resonance degrees of freedom in nuclei and nuclear matter. Using Argonne's massively parallel Chiba City and Jazz computer systems and the National Energy Research Scientific Computing Center IBM SP, the Laboratory's nuclear theory group has set world standards for calculations of nuclear many-body problems addressing fundamental questions in nuclear structure and nuclear astrophysics. The Argonne theory program provides important guidance for current and future experimental programs at ATLAS, TJNAF, and RHIC.

User Facility: Argonne Tandem-Linac Accelerator System

Situation

A DOE-designated national accelerator facility for research in nuclear physics, ATLAS employs beams of low-energy heavy ions. The accelerator provides high-quality beams of all the stable elements up to the heaviest, uranium. A recently completed electron cyclotron resonance ion source has increased beam intensity by an order of magnitude. ATLAS is based on a technology developed at Argonne that employs superconducting radio frequency accelerator cavities. The ATLAS facility serves a broad community of about 300 users from more than 40 research organizations and universities.

Vision

The ATLAS facility will operate reliably and provide its national community of users with unique heavy-ion beams for research at the forefront of nuclear, atomic, and applied physics. We will collaborate with U.S. industry to search for new applications of the superconducting radio frequency technology pioneered for ATLAS.

Objectives, Issues, and Strategies

The ATLAS program continues to optimize its operations and develop new linear accelerator technology to provide beams of higher intensity with excellent phase space and fast timing. Operational issues are reviewed continuously, and the facility's capabilities are enhanced frequently. We will be investigating technical and research issues relating to acceleration of beams of short-lived nuclei, as a basis for proposing development of a Rare Isotope Accelerator based on ATLAS. (See Section III.A.2.)

e. High-Energy Physics

Situation

We perform cutting-edge research on the physics of elementary particles and develop the instruments and accelerators needed to make that physics accessible. This work in high-energy physics leverages a range of diverse resources that generally are available only at a national laboratory. Our program includes four large experiments at different stages of preparation or data taking, a varied theoretical program, and R&D on advanced methods of particle acceleration potentially suitable for future research facilities.

Our researchers perform experiments at high-energy accelerator facilities in the United States and Europe. Other experiments are performed in special laboratory facilities without accelerators. In all projects, special attention is given to collaboration with university groups. This collaboration encompasses joint work on detectors and detector subsystems, as well as support for students working on theses in association with Argonne staff members.

Vision

To deepen and extend understanding of the physics of elementary particles, we will provide scientific leadership and will design and assemble major components of the required experimental systems. We will choose studies in theoretical physics for relevance to our experimental program or for general potential to advance understanding of interactions between elementary particles. Collaboration with universities will be emphasized.

Objectives

Major objectives of our work in high-energy physics are as follows:

- Maximize the output and impact of new physics generated from Argonne's experiments.
- Complete the demonstration of the Argonne Wakefield Accelerator and exploit the facility for further experiments in advanced acceleration technology.
- Advance the technology of detectors for high-energy physics by improving existing detector devices and inventing new ones.
- Improve theories of particle physics and expand understanding of experimental consequences.

Issues and Strategies

Experiments in high-energy physics are conducted in most cases by large international collaborations. Increasingly, accelerator or collider facilities are unique and are not duplicated elsewhere in the world. Accordingly, our work in high-energy physics is increasingly conducted at foreign accelerators, as well as at those in the United States. Data taking in the ZEUS experiment at the German DESY laboratory began in 1992, and ZEUS continues to provide unique data from high-energy electron-proton collisions. In 2001, a major luminosity upgrade was completed for ZEUS and related experiments, permitting a new focus on extreme values of kinematic variables where rates are low. Currently under way is fabrication work on a detector for the Large Hadron Collider (LHC), which is being constructed at the CERN Laboratory in Switzerland. Our researchers have established leadership roles in the ATLAS (A Toroidal LHC ApparatuS) detector, one of two major detectors planned for the LHC (and unrelated to the ATLAS facility located at Argonne). The U.S. government has a formal agreement with CERN that details the scope of U.S. participation in the LHC and the level of funding to be provided by DOE and the National Science Foundation. Some work on the ATLAS detector has shifted to preinstallation and installation activities that should be completed in 2005. The detector is expected to begin taking data in 2007.

We will be carefully considering expansions or new directions for many of our programs in high-energy physics, in order to preserve their effectiveness in the next decade. Our researchers are playing leading roles in the MINOS (Main Injector Neutrino Oscillation Study) experiment, a long-baseline study of neutrino oscillation, employing a neutrino beam from the new Fermilab main injector. MINOS is now in the installation phase. The "far" detector is underground, adjacent to the current Soudan 2 detector in Minnesota. We have built the major active components of the "near" detector (scintillator modules and electronics) and will be centrally involved in its installation and commissioning. First data from the detector are expected in FY 2005. A major upgrade of the Collider Detector at Fermilab began taking data with the upgraded Fermilab Tevatron in 2002. Our Wakefield Accelerator R&D program is now preparing for the second phase of its demonstration program; in order to explore ways of using this new accelerator technology in future experimental facilities, we are discussing possible collaborations and alliances with researchers at other institutions.

The ATLAS detector at the CERN Laboratory in Europe is designed to solve the fundamental puzzle concerning the mechanism of electroweak symmetry breaking and the origin of mass. Calorimeter fabrication began in FY 1999 and was completed at the end of 2002. Work on the calorimeter has shifted to a process involving preassembly and then installation of the detector at the CERN Laboratory. We are also currently contributing to the design and prototyping of the trigger for ATLAS. System components will be built, tested, and commissioned during the coming five years. Development of the computing system for the ATLAS detector began as a new task in FY 2000 and became fully integrated with other U.S. work on ATLAS during that year. In collaboration with other U.S. and foreign ATLAS institutions, we are taking the lead role in developing core data management software, as well as calorimeter-specific software.

In theoretical high-energy physics, funding limitations have prevented us from adding junior researchers at appropriate intervals. With DOE, we will explore means of adding one or more early career theorists, particularly in the area of neutrino physics.

Discussed below as a programmatic initiative is proposed R&D toward a linear electron-positron collider and an associated detector.

Initiative: Linear Collider Accelerator and Detector Technology

In January 2002 a subpanel of the DOE-National Science Foundation High Energy Physics Advisory Panel gave highest priority to construction of a linear electron-positron collider in the energy range 500-1,000 GeV. This collider will complement the LHC by having sensitivity to a similar energy and mass range for new phenomena but qualitatively different measurement and identification abilities.

Success in building and exploiting this new collider depends on resolving a number of design issues and choosing between two major accelerator technology alternatives, based on either warm or superconducting radio frequency cavities. Substantial R&D is also needed on the detector for the new collider, in order to optimize its ability to reconstruct events with the required precision. We plan R&D on both the accelerator and the detector. For the accelerator, we will use our world-class expertise in photocathode guns and electron beam optics. For the detector, we propose a new hadronic calorimeter technology based on resistive-plate chambers, which will be used with the energy flow approach to calorimetry being explored with the ZEUS detector.

Resources required for our work on this initiative are summarized in Table IV.3. Funding is sought from the DOE High Energy Physics Program (KA-04).

Table IV.3 Linear Collider Accelerator and Detector Technology ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	0.5	0.8	1.0	1.5	2.0	2.5	3.0
Capital Equipment	0.2	0.3	0.3	1.0	1.3	1.5	2.0
Construction	-	-	-	-	-	-	-
Total	0.7	1.1	1.3	2.5	3.3	4.0	5.0
Direct Personnel	2.0	4.0	5.0	8.0	11.0	13.0	15.0

f. Mathematics, Computing, and Information Sciences

Situation

In the 1980s and early 1990s more than 20 U.S. companies were producing supercomputers designed for scientific and technical applications. In recent years, however, that situation has changed. Scientific computing has become increasingly dependent on hardware designed and optimized for commercial applications. The performance of the Earth Simulator in Japan exposed the seriousness of this problem.

Typical scientific applications can extract only 5-10% of the power of supercomputers essentially built from commercial web and data servers. By contrast, the Earth Simulator makes 30-50% of its power accessible to most scientific calculations. By combining 40 trillion operations per second with optimization for scientific computing, the Earth Simulator gives its users a clear advantage over other researchers.

Regaining the U.S. lead in scientific computing will require dramatic advances in hardware, algorithms, systems software, and related enabling technologies. The hardware challenge alone is formidable. Current technologies, such as clusters and parallel vector processing, appear to be incapable of scaling effectively to the petaflops regime. Innovative computer architectures, such as virtual-vector and system-on-a-chip technologies, therefore must be explored. Critical to this effort will be sustained partnerships in which computer vendors interact directly with computer scientists and scientific applications teams throughout the prototyping, testing, and design of the new architectures.

Petaflops computing will also require a new software infrastructure. Simple enhancements to existing software will not suffice. Researchers will need to explore innovative strategies, such as linked development of systems software and compilers. Moreover, novel interfaces must be developed to integrate petaflops computing into emerging national computational grids, and high-level tools will be needed to enable users to move applications quickly and seamlessly from the workstation to a large-scale facility. A further major challenge will be the development of systems integration strategies to enable scaling of the system from teraflops to petaflops, while still using the same hardware and software elements.

Vision and Goals

We believe that it is possible, within a decade, to provide scientific computing in the United States with sustained performance increased by orders of magnitude. Key to realizing this vision is the development of world-class supercomputing and networking resources, complemented by world-class algorithms, tools, and software. Argonne, in collaboration with Berkeley Lab, is exploring a comprehensive new strategy that will couple scientific applications to the development of computer architectures. The goal is to open a sustainable path to petaflops-level performance and beyond.

Objectives

We have established the following specific objectives for achieving a world-class computing capability:

- Work with DOE to formulate a national strategy aimed at creating new computer designs that achieve maximum sustained performance on scientific applications.
- Form partnerships with applications developers, computer scientists, and hardware vendors, not simply to evaluate architectures, but to *drive* the design of new architectures by exploring design tradeoffs and testing early prototypes.
- Address key challenges to high-performance computing, including scalable input and output, fault-tolerant software, memory hierarchy management, performance analysis, and numerical and communication libraries.
- Spearhead development of the grid tools, middleware, and services needed for large-scale collaborative problem solving.
- Accelerate development and deployment of the ultrascale networks needed to complement the advanced architectures.

Issues and Strategies

Argonne researchers in the computing sciences are at the forefront of U.S. scientific computing. They lead efforts to develop new paradigms and technologies. For example, in collaboration with Berkeley Lab, we recently proposed to DOE a new program to accelerate scientific computing in the United States by implementing a radical new paradigm of collaborative development with computer vendors.

Of particular interest is the Blue Gene architecture, which potentially could scale far beyond current systems and enable researchers to attack key scientific problems in diverse disciplines. A software simulator is available now, and the vendor could provide a hardware simulator in late 2003 or early 2004; a full system of approximately 100,000 processors, capable of sustained petaflops computing speed, could be available by 2007-2008. To move forward, the vendor requires three major collaborators by the end of 2003. We are aggressively considering the possibility of participating.

In another important area of research — distributed computing systems — coupling workstations and parallel computers, large databases, virtual-reality devices, and other resources worldwide promises tremendous advances in scientific problem solving. Our deployment of the Globus Toolkit™ has made Argonne the center of distributed systems research worldwide. We are now exploring ways of extending this technology to areas of computational science such as a Proteomics Data Grid and a Biotechnology Data Grid. We are also taking the lead role in developing grid technology for many of the projects funded by the federal Scientific Discovery through Advanced Computing program, including the DOE Science Grid, the Earth Systems Grid, the Plasma Physics Collaboratory, and the Particle Physics Data Grid.

As a complement to these efforts in advanced computing, we have developed a major initiative in petaflops computing and computational science (see Section III.A.4). Central to this initiative is the development and deployment of a petascale experimental research facility that targets critical scientific problems. Argonne researchers have established a test bed and are exploring new technologies, such as cluster-on-a-chip, to enable computers to scale to systems capable of trillions of operations per second. The petascale facility primarily targets applications in the biosciences and nanosciences.

We have also established the Laboratory Computing Project to promote the widespread use of high-performance computing technologies for scientific research across the Laboratory. As part of this project, Argonne recently funded a teraflop-class computing cluster. This system was chosen because it is highly reliable and easily reconfigured, two features essential for heavy production. Early tests by nuclear physicists and astrophysicists have shown that the new system can achieve high performance on challenging computational science problems.

g. Intense Pulsed Neutron Source

Situation

The IPNS has operated as a national user facility since its commissioning in 1981. Among DOE neutron sources, it has one of the largest user programs: in both FY 2001 and FY 2002, 240-250 scientists conducted a total of approximately 400 experiments. The total number of participant scientists in 2002 was 680. Moreover, the IPNS is DOE’s most cost-effective neutron source. Its high scientific productivity and cost-effectiveness have been noted frequently by national and international committees. In February 2001 that evaluation was reinforced by DOE’s Basic Energy Sciences Advisory Committee (BESAC), which strongly recommended increasing annual IPNS funding by $9 million in order to (1) improve the accelerator, targets, moderators, and available instruments and (2) expand the facility’s research program. The IPNS currently provides 13 neutron scattering instruments, as well as facilities for studying radiation effects. The IPNS operated for 27 weeks in FY 2002, and it is scheduled to operate for 26 weeks in FY 2003.

Vision

The IPNS will function as a reliable and accessible user facility for neutron scattering research and as a successful developer of targets, moderators, and state-of-the-art neutron scattering instrumentation. Staff will help qualified users conduct world-class condensed matter research that addresses a wide range of questions important to both science and technology. Through enhancements, the IPNS will maintain leading-edge capabilities in neutron scattering. Through expanded collaboration with other Argonne facilities, such as the APS and the Center for Nanoscale Materials (CNM) (see Section III.A.1), the IPNS will further increase its scientific productivity.

Issues and Strategies

The IPNS has historically been severely oversubscribed, understaffed, and underfunded. The additional $4 million in IPNS operating funds included in DOE's Scientific Facilities Initiative beginning in FY 1996 now allows 26-27 weeks of operation per year, with a full complement of instruments serving users. A 16% increase in FY 2002 operating funds from DOE, along with an anticipated 7% increase in FY 2003, will enable us to begin work toward enhancing instruments. Improved instruments are expected to attract about 40% more users each year (340 rather than 240).

Neutron scattering in the United States will be in a state of flux for the next decade. Currently, two DOE facilities and a facility of the National Institute of Standards and Technology (NIST) provide neutrons to the user community: the IPNS, the Los Alamos Neutron Science Center (LANSCE) at Los Alamos National Laboratory, and the NIST Center for Neutron Research in Gaithersburg, Maryland. A major upgrade of the High Flux Isotope Reactor facility at Oak Ridge National Laboratory is currently under way, and construction of the 1.4-MW world-class Spallation Neutron Source (SNS), also at Oak Ridge, is scheduled for completion in FY 2006, with full user access scheduled for FY 2008. Consequently, over the next five years the IPNS will evolve from a major national source of neutrons for U.S. users to a medium-sized regional facility. In this environment, the role of the IPNS will be increasingly coupled to the APS and the CNM.

The role of the IPNS over the next decade in serving neutron scattering researchers and the broader scientific community is best described in terms of short- and long-term strategies.

Short-Term Strategies (Next Three Years). The IPNS role in the early transition period is to promote growth in the U.S. neutron user community and to support the SNS project to ensure the successful commissioning of that world-class facility. We also must begin positioning the IPNS for highly productive research after the SNS starts operations. These goals can be achieved through the following actions:

- Improve IPNS instruments so as to build the facility's user base (from 240 to 340) and train new neutron users more effectively.
- Contribute to the SNS project where appropriate, in the areas of target, moderator, and accelerator systems and user programs.
- Conceptualize SNS instrumentation capable of serving frontier scientific experiments in the coming decades.
- Leverage the full range of capabilities available at the CNM, the APS, and the IPNS in order to serve facility users better.
- Create joint staff appointments between the IPNS and the APS, the CNM, and the University of Chicago.

Long-Term Strategies (Beyond Three Years). Just before SNS operations begin, the IPNS role will be to begin development of the next generation of SNS instrumentation and to operate the IPNS with upgraded instrumentation that better supports the neutron scattering community. Closer ties with the APS and the CNM will facilitate more effective utilization of neutrons and photons to investigate fundamental issues in science and technology. We will also begin work on a new neutron source at Argonne to help support DOE's nanoscience initiative. These goals can be achieved through the following actions:

- Continue to operate the IPNS highly effectively (at 95% reliability).
- Give priority to development of IPNS instruments that will be capable of world-class science after SNS startup.
- Spearhead the design and construction of up to four SNS instruments. Commission and operate selected neutron scattering instruments at the SNS by using the concept of instrument development teams developed by the SNS.
- Further strengthen scientific ties to complementary U.S. facilities, starting with the APS and the CNM at Argonne. Establish further joint staff appointments with those Laboratory facilities.
- Develop designs for a new neutron source focused on serving nanoscience initiatives.

• Collaborate with other North American neutron centers in developing software and methods that support remote data access and control of experiments via the Internet.

Initiative: IPNS Enhancement

Under the IPNS Enhancement initiative, we propose to improve existing IPNS instruments significantly (increasing data rates by factors ranging from 2 to 32) and to increase the number of weeks of operation to enable an expanded user community to gain experience at a pulsed source in preparation for using the SNS. These additional operations and scientific capabilities were detailed in a plan presented to the November 2000 meeting of the BESAC subpanel reviewing operations at LANSCE and IPNS. In February 2001 our plan became the first of the subpanel recommendations approved by BESAC.

The performance of all IPNS instruments can be increased significantly through various enhancements, such as more detectors, better data acquisition systems, neutron guides, and new ancillary equipment. Implementation of these enhancements over the next four years will improve data rates by factors as great as 32, allowing many IPNS instruments to be competitive with those at the world's best pulsed neutron source, ISIS in the United Kingdom.

h. Biosciences

Situation

High-throughput DNA sequencing is providing a vast database of DNA information and, by inference, information about protein sequences across all kingdoms of life. The availability of these data means that biology has reached a turning point at which complete enumeration of the genes used by any organism is within easy reach. The challenge now is to interpret this information to construct a detailed, coherent, complete view of living organisms and to use this view to develop methods for manipulating and engineering biomolecular systems and predicting their responses to environmental stimuli. The key to such detailed control of biomolecular systems lies in a complete mapping of the activities of the gene products of a cell that cooperate to perform all cellular processes. The information required to characterize these processes is embedded in the spatiotemporal distribution of gene products and metabolites across multiple length scales.

In coming years, progress in the biological sciences will depend increasingly on inter-disciplinary interactions with computational, physical, chemical, and materials scientists. Implementation of high-throughput techniques for biochemical and biophysical characterization of biomolecular systems will make it possible to address experimental challenges that are now unbroachable. Huge volumes of data will be required. Cataloging and preserving those data and then extracting maximum information will present a significant challenge in database design and maintenance. In the longer run, integrating the data into a complete view of cellular (and, ultimately, organismal) behavior will require novel approaches to simulating complex systems. Computation will come to dominate the biological sciences in the 21st century. This approach to genome-scale analysis of biological function, now widely referred to as systems biology, involves the fusion of functional genomics with high-end computational simulations of the molecular behavior within biomolecular systems.

Vision and Goals

We will move toward a leadership position in postgenomic biology by creating a model program for the comprehensive functional analysis of genomes. The Functional Genomics initiative (see Section III.A.3) will take advantage of our strong programs in the physical, chemical, materials, and computational sciences to build, along with biosciences, a uniquely interdisciplinary program for postgenomic biology. Partnership with computational scientists will develop a systems biology capability that will be well positioned for the comprehensive analysis of the behavior of microorganisms that are relevant to DOE's science mission.

Experimental facilities at the APS and world-class computational resources will be integral parts of our program for genome-wide structural and functional characterization of organisms — a program that will be centered around our quickly growing effort in structural and functional genomics. Revolutionary approaches to currently intractable problems will be explored in collaboration with Argonne physicists, chemists, and engineers. Programs in bioinformatics, nanobiotechnology, and combinatorial biology will engage scientists at both the Laboratory and the University of Chicago. The goal is a focused program aimed at developing and using high-throughput experimental and cutting-edge computational capabilities for the complete functional characterization of whole genomes.

Objectives

Our Functional Genomics initiative will grow around our current structural and functional genomics programs by taking advantage of both resources supporting the current program and other resources at the APS and across the Laboratory. The initiative will greatly strengthen cross-disciplinary interactions aimed at creating revolutionary approaches to currently intractable problems.

Our major objectives in biosciences are focused on the major Laboratory initiative Functional Genomics (Section III.A.3), elements of which include the following ongoing and novel efforts:

- *Structural Genomics.* Develop a scientific program aimed at deepening understanding of the relationship between protein structure and function — a program centered on current efforts to characterize to atomic resolution the three-dimensional structure of all gene products and to use that structural information to develop better understanding of the function of each gene product.

- *High-Throughput Protein Production and Crystallization.* Our current use of robotics for high-throughput expression of proteins will provide milligram quantities of hundreds of proteins for functional analysis. In parallel with crystallization efforts, these proteins will be analyzed by using functional proteomics, combinatorics, and x-ray solution scattering. The robotics expertise of our scientists will be exploited to develop techniques for high-throughput biochemical and biophysical analyses. Upgraded robotics capabilities for the rapid and efficient production of diffraction-grade crystals of biological macromolecules will eliminate the most severe bottleneck in our structural genomics work.

- *Revolutionary Approaches to Membrane Protein Crystallization.* The 30% of proteins that are integral components of cellular membranes cannot be investigated with the techniques that are successful in crystallizing other proteins. In collaboration with physical and chemical scientists, we will explore revolutionary approaches to the crystallization and biochemical analysis of these proteins.

- *Program for Combinatorial Biology.* Mapping of protein-protein and protein-ligand interactions is one of the most powerful methods for the functional analysis of macromolecules. A comprehensive program in combinatorial biology is being developed to take advantage of the huge potential of this approach for the functional analysis of whole genomes. Furthermore, a program for the high-throughput production of affinity tags will be developed to aid in the purification and functional analysis of gene products. This program will use vast libraries of proteins and peptides displayed on the surfaces of viruses and bacteria and will screen these libraries for desired functionalities.

- *Program in Nanobiotechnology.* Our materials scientists and biologists will cooperate to develop a new program in nanobiotechnology that will explore the creation of bio-inspired nanostructures and bio-compatible materials, as well as the structural analysis of complex biological materials.

Issues and Strategies

We are uniquely positioned to take advantage of the extraordinary opportunities developing in postgenomic biology. Through multidisciplinary collaborations among scientists across the Laboratory and at the University of Chicago, we will seek leadership in newly defined areas of the biological sciences and will explore revolutionary approaches to a number of currently intractable problems in structural and cellular biology.

The core of our bioscience efforts is work in structural genomics to establish high-throughput macromolecular crystallography and its use for enumerating all existing protein structural motifs. This work has motivated initiatives in high-throughput crystallization of macromolecules and high-throughput expression of proteins in bacterial hosts. Building on our existing robotics expertise, these initiatives will provide a further base for developing robotics for rapid biochemical and biophysical assays of protein structure and function. Our existing structural genomics efforts are tightly focused on crystallographic studies, and augmentation in the indicated directions is a priority.

In general, development of new interdisciplinary interactions across the Laboratory and with the University of Chicago will drive our planned initiatives in the biosciences, where DOE and the National Institutes of Health (NIH) will be major funding sources. The Functional Genomics initiative (Section III.A.3) directly addresses the goals of DOE's Genomes to Life program. In addition, important funding from the state of Illinois is being sought to enhance the planned program in high-throughput protein production and crystallization. A key complementary strategy is development of cooperative agreements with biotechnology companies for joint development of novel methodologies.

Our initiatives in the biosciences will build from four parallel and complementary efforts in macromolecular crystallography that are currently being pursued: (1) the capabilities of the existing DOE-funded Structural Biology Center are being enhanced significantly through support from NIH. The Midwest Center for Structural Genomics receives from NIH approximately $5 million per year for development of high-throughput macromolecular crystallography. (2) In partnership with this effort, we are also working with NIH to develop a second APS sector for macromolecular crystallography. (See Section S1.C for discussion of these NIH-supported efforts.) (3) To facilitate this work, a laboratory complex for biostructure research has been constructed at the APS with joint DOE and NIH funding (see Section IV.A.1.a). (4) We are also working with the state of Illinois on plans to construct an Accelerated Protein Production and Crystallization Facility at the APS, which is to include development of an additional APS sector for structural genomics and macromolecular crystallography. Close partnerships among these four efforts will enable significant economies of scale, facilitating rapid improvement in the understanding of structure and function in proteins.

We are building our Functional Genomics initiative around these significant efforts in structural and functional genomics and crystallography. Research on genome-wide analysis of the structure, assembly, and operation of gene products is greatly expedited by the use of large-scale, high-throughput capabilities for analyzing intermolecular interactions and other biochemical and biophysical parameters of macromolecular complexes. This initiative will establish the resources needed for comprehensive studies of biomolecular machines, interface this effort with our ongoing work in structural genomics, and use the resulting capabilities to characterize the molecular machines critical to cellular processes in all organisms.

i. Environmental Research

Situation

Environmental research at Argonne comprises three intersecting thematic areas reflecting the unique role that Argonne and the other national laboratories play in accomplishing DOE's missions. Argonne's basic research strengths in atmospheric, molecular, and terrestrial sciences are complemented by our successful operation of environmental research user facilities and by our development of new methods and technologies for applied and basic environmental studies. Our multidisciplinary research approach, active collaborations with academic partners, and the ability to assemble and operate complex laboratory and field-based user facilities have allowed us to enhance our own research and foster the work of the broad environmental research community.

Vision

We expect to be a leading institution for assembling the flexible, interdisciplinary teams required to address the nation's high-priority environmental problems. Our work will aim at integrating state-of-the-art advances within disciplines — in such diverse areas as structural biology, atmospheric chemistry, functional genomics, climate science, global carbon cycling, and environmental molecular science — with cross-disciplinary system-level studies to improve understanding of how humans and other living things interact with and respond to their environments.

Mission, Goals, and Objectives

The primary mission of Argonne's environmental research program is to perform and facilitate world-class research in the areas most important for addressing high-priority environmental problems critical to the interests of DOE and the nation.

Our overall goals are as follows:

- Optimize the efficiency and enhance the capabilities of the Climate Research Facilities of the Atmospheric Radiation Measurement (ARM) Program (supported by DOE's Office of Biological and Environmental Research [DOE-BER]).
- Extend environmental research activities at Fermilab, at the Atmospheric Boundary Layer Experiments (ABLE) site, at the ARM Climate Research Facilities, and at other field sites to serve diverse user communities investigating air-surface exchange, boundary layer dynamics, carbon cycling, climate science, ecosystem processes, and nutrient dynamics across a range of spatial scales.
- Develop synchrotron-based capabilities that use the high-brilliance x-rays of the APS for molecular-level investigations of environmental systems and atomic-scale studies of mineral-fluid interfaces.
- Establish cross-disciplinary interactions with other Laboratory researchers in the areas of computational science, functional genomics, materials science, and nanoscience, in order to pursue solutions to significant new environmental challenges.
- Expand our interactions and collaborations with the University of Chicago and other academic partners in the areas of atmospheric science and molecular environmental science.
- Optimize the productivity of scientists conducting research at the interfaces between the scientific disciplines relevant to addressing environmental issues.
- Increase the size of our base scientific program.

Among our specific objectives for FY 2004 are the following:

- Redirect our existing strengths in atmospheric chemistry and physics toward new research on the climatic effects of atmospheric aerosols.
- Complete formation of the multi-institutional EnviroCAT consortium and secure approval from the APS Science Advisory Board for a new APS sector devoted to environmental science.
- Define a staff position and offer it to an environmental microbiologist who can contribute to our current work in terrestrial ecology, molecular science, and bioremediation and also can apply new discoveries in functional genomics to enhance understanding of environmental processes on real-world scales.
- Consolidate and extend our participation in the joint Argonne–University of Chicago Center for Environmental Sciences by establishing an Urban Atmospheric Observatory focused on the effects of urbanization on regional climate variability and human health.

Issues and Strategies

The major challenges facing Argonne's environmental research program are to maintain a distinguishing institutional identity and to continue to serve as a uniquely valuable resource to DOE. Competition from universities and industry for qualified staff and new research programs, along with loss of DOE base funding for environmental science, has exacerbated the difficulty of recruiting and retaining a first-class professional workforce. It has also led to a dated research infrastructure in some areas and increased pressure to pursue research opportunities that may be peripheral to the Laboratory's primary scientific interests.

We nevertheless remain convinced that Argonne and the other national laboratories will continue to play an important and unique role in addressing the nation's environmental research needs. The future of environmental research at the national laboratories lies in increased emphasis on basic and applied research conducted by multidisciplinary teams that can fully exploit major research facilities and other unique capabilities. Our general strategy, therefore, is to leverage our existing strengths by reaching across traditional disciplines to integrate environmental research that ranges in scale and hierarchical organization from the molecular to the regional.

Climate Change. Among DOE's priorities in climate change research are (1) understanding the factors affecting Earth's radiant energy balance, primarily through the ARM Program; (2) through the DOE-BER Climate Change Prediction Program (CCPP), accurately predicting regional and global climate change induced by increasing atmospheric concentrations of greenhouse gases; and (3) through the Terrestrial Carbon Processes (TCP) program, quantifying the sources and sinks of energy-related greenhouse gases.

Although we manage the ARM facilities and the ABLE site for the ARM Program and are leading the transition of those sites to national user facility status (as ARM Climate Research Facilities), our scientific research in the ARM Program is not supported commensurately. DOE-BER recently redirected its Atmospheric Science Program toward study of the radiative effects of atmospheric aerosols, offering us a new opportunity to increase our scientific work in this important area of atmospheric research. Improving understanding of atmospheric aerosols is therefore one of the major thrusts of the Laboratory's Challenges in Environmental Science initiative, described in more detail below. This initiative proposes to bring together Argonne's atmospheric scientists, chemists, and materials scientists in an interdisciplinary effort to develop a predictive understanding of the contribution of aerosols to Earth's radiation balance. By coordinating theory, laboratory, field, and modeling work across these disciplines, we will seek new knowledge relating aerosol formation, transformation, and transport to radiative processes that occur on urban, regional, and global scales. This work will intimately involve Argonne computer scientists who have already made substantial contributions to the CCPP. Because performance improvements gained by applying advanced computing are worthwhile only to the extent that real-world processes are represented accurately in the models, we propose to establish firmer connections between scientists studying the atmosphere and those working in the computer laboratory.

Our TCP work is tightly linked to our ongoing research in soil ecology, which aims specifically at understanding carbon cycling in soils and, through the DOE-BER Carbon Sequestration in Terrestrial Ecosystems consortium, at quantifying the potential for carbon sequestration in soils representing different ecosystems. By using combinations of field studies and carefully selected supplemental laboratory experiments, scientists in our terrestrial ecology program have pioneered understanding of the complex belowground ecosystem. Our objective now is to link our work with new DOE-BER programs in functional genomics by taking advantage of new technologies and facilities for the study of basic biogeochemical processes. We see the opportunity to use genomic methods to design and develop environmental "transponders" that could be valuable tools for understanding the responses of whole ecosystems to global environmental change. This work is also linked to our research in environmental remediation and basic biogeochemical cycling, which is described below.

Global changes are caused by multiple factors, so it is unproductive to study carbon cycling in isolation. We therefore plan to draw on our experience in terrestrial ecosystem research and our expertise in atmospheric sciences to develop a companion program aimed at nitrogen cycling. (This work is also part of our Challenges in Environmental Science initiative.) The first objective is to develop an effective methodology for investigating interactions of the carbon and nitrogen cycles in the field. We expect this research area to grow substantially as better techniques for studying atmospheric and terrestrial processes evolve, and we plan to be among the leading institutions working at conceptual interfaces between disciplines and at physical interfaces between atmospheric and terrestrial systems.

Environmental Remediation. The primary goal of our work in synchrotron-based environmental science is to increase atomic- and molecular-level understanding of structures and processes in environmental systems. One set of studies considers mineral-fluid interactions and the mechanisms by which contaminant elements become bound to mineral surfaces. Another set of studies focuses on developing synchrotron-based imaging techniques for environmental and biological samples and on understanding the speciation, binding, distribution, and mobility of heavy metals and radionuclides in soil-fluid-biota systems. These multidisciplinary efforts build on our recognized achievements in molecular radiation and environmental science, and they involve several new internal and external collaborations. Expanding our capabilities for this work is a key component of the Challenges in Environmental Science initiative.

Initiative: Challenges in Environmental Science

Argonne's research in many areas has significant potential for beneficial application in environmental science. Through multidisciplinary teams we propose to address two nationally recognized environmental "grand challenge" phenomena that are especially compatible with our expertise and facilities: (1) biogeochemical cycling, particularly cycling of iron and nitrogen, and (2) atmospheric particulates and aerosols. We also plan to develop a new facility for synchrotron environmental science to enable other aspects of the initiative.

In the area of *biogeochemical cycling*, central goals are to (1) quantify the rates of transfer of compounds to and from storage reservoirs and (2) determine the mechanisms controlling these transfers. The most important challenges are to understand how Earth's major biogeochemical cycles are perturbed by human activities; to predict the impact of these perturbations on local, regional, and global scales; and to determine how these cycles could be restored to more natural states. Argonne teams will focus on primary and secondary interactions among the multiple elements of these problems and on associated positive and negative feedbacks. Studies will range from the atomic level to bench scale to field scale.

Atmospheric particulates and aerosols, both natural and anthropogenic, are inextricably linked to energy production and use. Such particles have significant detrimental effects on human health, play a major role in acid rain formation, and have direct and indirect radiative forcing effects that are comparable in magnitude to the effects of greenhouse gases but are opposite in direction. The characteristics, distribution, and transport of such particles over long distances affect issues ranging from national security (e.g., the transport of harmful spores) to general air quality (e.g., atmospheric chemical interactions). Our research will determine how atmospheric particles are formed, their roles in global and regional climate systems, and their relevance to chronic and acute respiratory diseases. Approaches based on materials science, chemistry, and physics are particularly appropriate for these studies.

To meet the growing need for additional capabilities in *synchrotron environmental science*, we have formed a partnership with the University of Notre Dame and the U.S. Environmental Protection Agency to establish a new APS collaborative access team devoted to environmental research. This "EnviroCAT" aims to provide dedicated, state-of-the-art facilities optimized for research on a broad range of environmental science problems. EnviroCAT will focus on developing a multifaceted microbeam facility and a microtomography facility that use, respectively, insertion device beamlines and bending magnet beamlines. The APS program review board has approved the EnviroCAT letter of intent, and a formal proposal was submitted and reviewed in January 2003. In FY 2004 we expect that work to develop initial design criteria will begin and that discussions with potential institutional partners will result in additional formal research partnerships.

Proposed work on *biogeochemical cycling* and *atmospheric particulates and aerosols* fits within the scope of the initiative in climate change of the U.S. Global Change Research Program, which is a likely near-term source of funding. Other programs that would benefit from our pioneering approach to multidisciplinary integrated research are the DOE-BER Genomes to Life program and

DOE’s environmental remediation studies, such as those of the Natural and Accelerated Bioremediation Research program and the Environmental Management Science Program. These efforts will draw on the new Joint Argonne–University of Chicago Center for Environmental Science, a formal collaboration to investigate significant environmental issues. Other potential federal sponsors are the Environmental Protection Agency, the National Oceanic and Atmospheric Administration, the National Aeronautics and Space Administration, the National Science Foundation (through collaborations with university partners), and the Department of Defense.

Required resources are summarized in Table IV.4. Also reflected in the table are resources envisioned for work in *synchrotron environmental science* and for developing EnviroCAT (including construction). As indicated above, support will be sought from DOE-BER (KP), other federal agencies, and private sources.

Table IV.4 Challenges in Environmental Science
($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	0.6	2.0	3.6	5.6	8.0	10.0	10.0
Capital Equipment	-	2.5	2.5	2.5	2.0	2.0	2.0
Construction	-	8.5	4.0	4.0	-	-	-
Total	0.6	13.0	10.1	12.1	10.0	12.0	12.0
Direct Personnel	3.0	5.0	9.0	14.0	20.0	25.0	25.0

j. Science and Engineering Education and University Programs

Situation

Through the years, Argonne has consistently maintained very active and wide-ranging interactions with the academic community. These activities range from programs that support science education at the high school level to mutually beneficial research partnerships between university faculty and Argonne research staff in virtually all of our scientific and technical areas. The activities are supported by the Laboratory, through work for non-DOE sponsors, and by DOE.

Our science and engineering education programs serve faculty and students at both the university and precollege levels. Core programs at the university level provide opportunities for research participation by outstanding undergraduates and faculty, as well as opportunities for thesis research by graduate students. We have become more active in unique graduate programs involving several strategic areas of interest to DOE. These programs include long-term internships and short-term training in a wide range of our research areas. The quality and value of these programs attract applicants from throughout the country.

As part of our education program, we serve the Department of State as the host institution for U.S. participation in training programs of the International Atomic Energy Agency (IAEA). In FY 2002, our role expanded to include placement of IAEA fellows in R&D environments throughout the country. As in earlier years, we have continued to develop and conduct courses in peaceful applications of nuclear technology and also to provide technical support to the Department of State and the IAEA.

Vision

We will enrich science education in the United States through activities that involve local communities, as well as students and faculty at all levels from throughout the nation. We will work closely with DOE and other federal agencies to promote peaceful applications of nuclear technology through collaboration with the IAEA and other international organizations.

Objectives

Our primary near-term objectives in support of science education and training are as follows:

- Continue to attract a large, diverse pool of highly qualified undergraduate students to research participation programs.
- Establish our educational user facility as a valuable and widely used resource providing hands-on laboratory experience for science teachers from the region and throughout the

country; enhance classroom activities through use of the Internet.

- Foster student interest in science education and science careers through a variety of outreach efforts.
- Fruitfully integrate graduate students, post-doctoral fellows, and faculty into Laboratory research programs through internships and training activities.
- Provide training programs and technical assistance to a variety of international organizations.

Issues and Strategies

For our university-level programs, we plan special efforts to develop supplementary activities that will broaden the science horizons of undergraduates and provide training and research opportunities for graduate students. Programs for high school students and teachers will focus primarily on hands-on laboratory work using Argonne facilities and distance learning capabilities dedicated to educational activities. In addition, we will continue to develop programs exploiting computer technology to enhance classroom science education. Important work-shops and conferences, such as the annual Women in Science conference, will continue. International programs will focus on unique Argonne research and training capabilities.

Maintaining a sound funding base is the most important issue currently facing our educational programs. Support for participants through the Office of Science has included limited infra-structure support. DOE offices with educational and training needs have been asked to consider the advantages of focusing those activities at Argonne. Our research divisions plan to continue their strong support for the core educational programs of research participation and thesis research at the undergraduate, graduate, and faculty levels. Support for the operating costs of programs for precollege teachers will be sought from the state of Illinois, agencies of the federal government, and the private sector. Laboratory overhead will support the minimal infrastructure required to manage and administer these programs.

2. Energy and Environmental Technologies

Argonne research programs serving the two DOE mission areas of energy and environmental quality are intertwined; this section includes area plans related to both.

a. Advanced Nuclear Technology

Situation

The May 2001 report of the National Energy Policy Development (NEPD) Group chaired by Vice President Cheney summarized its endorsement of nuclear power as follows: “The NEPD Group recommends that the President support the expansion of nuclear energy in the United States as a major component of our national energy policy.” The NEPD Group further recommended reconsideration of next-generation advanced-fuel-cycle technologies: “In the context of developing advanced nuclear fuel cycles and next generation technologies for nuclear energy, the United States should reexamine its policies to allow for research, development, and deployment of fuel conditioning methods (such as pyroprocessing) that reduce waste streams and enhance proliferation resistance.”

In view of these and other recommendations of the NEPD Group, we plan to accelerate our efforts to advance nuclear technology, in order to ensure that nuclear energy can fulfill its promise as a sustainable, clean, safe, long-term energy source, free of carbon dioxide emissions. To this end, we propose in Section III.B.1 the major Laboratory initiative Advanced Nuclear Fuel Cycle. At the conclusion of this area plan, we also propose expansion of our existing R&D on nuclear technology, which supports current nuclear technologies, as well as those of the near future and the longer-term future.

For more than a half century, we have been a world leader in the development of nuclear energy. Our staff has extensive expertise in the full range of disciplines associated with nuclear reactor technology, and a full complement of experimental facilities is in place, representing many hundreds of millions of dollars of national assets. Currently, our nuclear technology R&D focuses primarily on (1) the Advanced Fuel Cycle

Initiative, which aims to close the nuclear fuel cycle with new technology that is environmentally sound, proliferation resistant, and economical; (2) the Generation IV R&D program, whose objective is a new generation of nuclear reactors for deployment before 2030; (3) the Nuclear Energy Research Initiative (NERI), which involves work on innovative reactor concepts and on nuclear science and technology; and (4) operation of the International Nuclear Safety Center, which improves the safety of nuclear reactors worldwide through collaborative R&D programs and in-depth safety analysis, with primary attention to Soviet-designed reactors and the countries operating those reactors.

In partnership with the Idaho National Engineering and Environmental Laboratory (INEEL), we serve as lead laboratory for Nuclear Reactor Technology for the DOE Office of Nuclear Energy, Science and Technology (DOE-NE). In July 2002 the Secretary of Energy designated Argonne-West and INEEL as technical leads for the Advanced Fuel Cycle Initiative and the Generation IV program.

Goals

The goals of our nuclear technology program are to develop and demonstrate innovative nuclear reactor systems and associated fuel cycles that will ensure that nuclear energy can fulfill its promise as a sustainable, long-term, emission-free source of energy; to aggressively pursue solutions for the important technical issues associated with the use of nuclear energy, both domestically and internationally; to help DOE identify and implement technology development programs that will increase the contribution of nuclear energy to a sustainable global energy supply and to the production of hydrogen and fresh water; and to maintain a set of technical capabilities in nuclear science and technology — including both expertise and infrastructure — sufficiently broad and deep to address a full range of national needs.

Strategies

Key strategies for our nuclear technology programs include the following:

- Undertake the major Laboratory initiative Advanced Nuclear Fuel Cycle, including nuclear system R&D and design studies carried out in concert with the Generation IV program and the demonstration of an advanced fuel cycle. (See Section III.B.1.)
- Establish a major Laboratory initiative to investigate the production of hydrogen by nuclear energy. (See Hydrogen Research and Development in Section III.B.2.)
- Develop a space nuclear reactor initiative that responds to the expressed interest in fission reactors for space missions of the National Aeronautics and Space Administration.
- Continue to participate in the NERI, NEPD, and Generation IV programs; apply Argonne's nuclear expertise and unique facilities to current, near-term, and longer-term future nuclear technologies; and apply our expertise to critical issues affecting the continued safe and efficient operation of existing nuclear power plants.
- In partnership with INEEL, serve as lead laboratory for reactor technology for DOE-NE.
- Within our areas of special expertise, participate in advanced technology R&D programs such as the Advanced Fuel Cycle Initiative and nuclear security programs.

Argonne plans a number of important new directions for its work in nuclear R&D that will support the above strategies:

- *Transient Testing at TREAT*. We have begun work to reactivate the Transient Reactor Test Facility (TREAT) in order to carry out various experiments requiring a reactor capable of producing controlled transients. Though TREAT can be restarted, potential future testing missions will require additional resources. These missions might include testing the safety of fuel containing recycled actinides, testing the safety of advanced fuel concepts that might arise from the Generation IV program, or testing current or new fuel designs for commercial light-water reactors.

• *Advanced Fuels Development*. We propose to develop advanced fuels for power reactors, research reactors, and test reactors. Programs such as NERI and Generation IV have fostered discussion of various system configurations, but a common feature is a new fuel design. Of particular interest are metal and metal matrix dispersion fuels. Guided by system studies and technology road maps, we will pursue these fuel development options and others.

• *Materials Development for Nuclear Power*. Materials R&D is important for supporting the current fleet of operating nuclear power plants, as well as for developing future innovative nuclear systems. Future nuclear power plants are likely to operate at higher temperatures and have unique corrosion environments, so advanced structural materials will be necessary. We will undertake both fundamental and applied work to (1) investigate improvements in the performance and production of materials potentially applicable to nuclear power, (2) establish the capability to use modern production and analytical techniques, (3) screen new materials for likely performance in a nuclear environment, and (4) perform prototypic testing of promising advanced materials. Research aimed at both near-term and longer-term applications is proposed.

• *Post-Operation Evaluation of EBR-II Materials and Components*. A complete knowledge of the condition of Experimental Breeder Reactor-II (EBR-II) materials and components will facilitate future reactor decommissioning, life extension for current reactors, and the design of advanced reactors. In order that these valuable data not be lost, we propose significantly expanded examination of EBR-II materials and components.

• *Severe-Accident Management Technology*. Severe-accident research addresses the question of what could be done at a nuclear power plant if a core melt accident were to occur. Argonne's facilities for conducting severe-accident experiments have been designated an international reactor safety R&D facility by the Organization for Economic Cooperation and Development (OECD). A new research program investigating interactions between concrete and a molten reactor core is now under way. We seek continued funding for this program, whose costs are shared with international partners under OECD auspices. (See Section S1.E.5.)

• *Advanced Modeling and Simulation for Nuclear Applications*. We propose expanded work in advanced modeling and simulation for nuclear technologies. The first part of this work focuses on developing and implementing numerical methods on state-of-the-art parallel computers and workstation clusters, so that today's computing technology can be applied to improving nuclear reactor analysis. The second part focuses on machine reasoning, automated pattern recognition, and system modeling based on learned input-output relationships.

• *Space Nuclear Power*. DOE's work on radioisotope power systems includes the development, assembly, testing, and supply of systems for application to the exploration of deep space and to national security. At Argonne-West we recently began contributing to this program by performing final assembly and testing for radioisotope thermoelectric generators. This new activity takes important advantage of our core competencies in nuclear research and strongly complements existing Argonne programs. Future related work could include R&D on advanced radioisotope power systems and on fission systems for propulsion in deep space.

b. Energy and Industrial Technologies

Situation

We develop innovative, efficient, cost-effective nonnuclear energy technologies and industrial technologies. Emphasis is on advanced transportation (discussed separately in Section IV.A.2.c), "industries of the future" identified by DOE, superconductivity, and fossil fuels and carbon management. The Energy and Industrial Technologies program also coordinates the Laboratory's development of partnerships with private companies in these areas.

Industries of the Future. Process industries convert raw materials into ingredients useful for fabrication and assembly in the automotive, electronics, aerospace, construction, and similar industries. The process industries account for approximately a third of U.S. energy consumption, at an energy cost of about $100 billion each year. Six of the major process industries — chemicals, forest products, glass, ceramics, metals, and petroleum refining — account for 78% of all industrial energy use, generate 95% of manufacturing waste, cause 95% of the total air pollution attributable to manufacturing, and account for more than 30% of U.S. carbon dioxide emissions. Because they use so much energy and produce so much waste, the federal government has set goals for U.S. process industries for the year 2010 in terms of energy reduction, oil displacement, cost savings, and pollution reduction.

Superconductivity. The electric power industry today faces a wide range of major challenges, including deregulation, aging infrastructure, global warming policies, and dependence on imported oil. Power wheeling across long distances puts a premium on technologies for the transmission and distribution of electric energy that are efficient and robust, and greater interconnectedness necessitates better technologies to protect against overloads and fault currents. Renewable energy sources are increasingly attractive, but solar or wind energy is intermittent and requires energy storage. High-temperature superconductivity technologies are being pursued by DOE and by increasing numbers of electric power utilities and their suppliers as a promising response to many of these challenges.

Fossil Fuels and Carbon Management. A prudent carbon management strategy for the utility, industrial, and transportation sectors could significantly decrease net emissions of carbon dioxide and other greenhouse gases. An early, economical opportunity for greater sequestration may be provided by the capture of carbon dioxide at large point sources such as power plants, followed by use for enhanced oil recovery and production of methane from coal beds. Sectors of the economy that consume large quantities of fossil fuels are already adopting more energy-efficient technologies. Strategies for the economical use of less-carbon-intensive fuels in existing plants and fleets may be an important bridge to more advanced technologies. However, a full assessment of policy options will require better understanding of carbon transformations "from cradle to grave," throughout current and proposed energy cycles. Our research initiatives support DOE strategies to improve the efficiency of fossil energy technologies and to assist the utility, industrial, and transportation sectors in reducing greenhouse gas emission rates in other ways as well.

Partnering. Responding to the administration goal of improving the productivity of U.S. industry through appropriate use of national technical resources, we are developing a broad range of partnerships with industrial firms on the basis of our leadership in many areas of science and technology. Argonne's midwestern location in the nation's industrial heartland provides exceptional regional opportunities. Partnerships with industry play an important role in shaping many Laboratory R&D programs.

Vision

We will develop new technologies that increase the productivity of U.S. industry and decrease its environmental impacts, particularly through increases in energy efficiency and reductions in intensity of petroleum consumption. As an integral part of pursuing our mission in science and technology, we will continue to develop effective relationships with industry to maximize the commercial applications and benefits to the nation from our R&D.

Goals and Objectives

To implement this vision, Argonne's goals include the following:

- Exploit and expand our facilities, capabilities, and core competencies, which integrate science and technology and interest both the scientific and industrial communities.
- Establish strategic partnerships with key industrial firms, large and small, in areas where applying our technical strengths is most likely to lead to valuable commercial successes.

• Implement effective regional outreach, capitalizing on our midwestern location.

Many U.S. industries are working with the federal government to ensure that federally sponsored R&D provides maximum benefits to the nation. We have established the important research objectives summarized below and are pursuing them in close partnership with industry.

Industries of the Future

• Expand Argonne research benefiting the chemical industry, particularly research in the areas of recovery and reuse of polymers, development of chemicals from alternative feedstocks, separative bioreactors, catalysis, and plasma-chemical engineering.

• Work with an industrial equipment supplier and a paper industry manufacturer to develop the multiport dryer technique, already demonstrated through proof of concept, into a prototype demonstration unit.

• Maintain the momentum of current research on metals recycling; expand work on instrumentation, materials, and fabrication technologies for the steel, aluminum, glass, and metal casting industries.

• Target key technical hurdles where unique Argonne capabilities and facilities can be used to advantage; for example, use the APS and the IPNS for critical materials studies that will enable the development of inert metal anodes for aluminum smelting.

• Advance the development of nearly frictionless, nontoxic carbon and nano-crystalline diamond coatings for moving parts (such as oilless bearings, spacecraft mechanisms, rolling and sliding gear systems, and bearings for ultrahigh-vacuum instruments like x-ray tubes), while contributing more broadly to tribology.

• Expand our research benefiting the glass industry by means of multiphase computational fluid dynamics modeling of glass furnaces; develop new techniques for recycling glass with minimal effect on product quality.

Superconductivity

• Maintain core work on the development of superconductors that is sufficiently broad to sustain rapid technical development and foster extensive interactions with industrial companies and universities.

• Continue our contributions to the development of the second generation of high-temperature superconductors, building on earlier successes with powder-in-tube technology.

• Work with the manufacturers of high-temperature superconducting wire (such as American Superconductor Corporation, IGC-SuperPower, and Universal Energy Systems, Inc.) to help advance manufacturing processes.

• Collaborate with system manufacturers (such as Boeing, IGC-SuperPower, and S&C Electric Company) to develop and demonstrate energy-efficient products for the electric power industry, such as flywheels for energy storage, fault current limiters, and transmission cables.

• Collaborate with other national laboratories and industrial partners to develop textured buffer layers — such as MgO, YSZ, Y_2O_3, and CeO_2 — for yttrium-based superconductor films.

Fossil Fuels and Carbon Management

• Expand and help coordinate the development of technologies that are cost-effective and highly efficient, emit smaller net amounts of greenhouse gases, and reduce environmental impacts in the utility, industrial, and transportation sectors; establish emissions inventories for promising technologies and form industrial partnerships to pursue technology development.

• Advance petroleum refining technology by developing (1) catalysts for upgrading heavy crudes, residuum, and distillates and (2) catalytic processing to produce ultraclean low-sulfur transportation fuels through heteroatom removal.

- Investigate opportunities for sequestering carbon dioxide derived from advanced fossil fuel energy systems and from retrofitting technology to the large number of existing long-lived electric generation plants.
- Improve understanding of terrestrial and oceanic responses to natural and anthropogenic changes in atmospheric concentrations of greenhouse gases.
- Develop a center for research on biogeochemical cycling of elements.
- Expand R&D on noncarbonaceous hydrogen production. (See the major Laboratory initiative Hydrogen Research and Development in Section III.B.2.)
- Extend Laboratory breakthroughs in ceramic membrane technologies to advance the development of economical processes for separating oxygen from air and hydrogen from mixed gases (which are critical technologies in, respectively, the use of remote natural gas and the efficient refinery production of clean transportation fuels).

Issues and Strategies

Industry. Through the auspices of the DOE Office of Industrial Technologies, we are working closely with the following industry associations to apply our skills, facilities, and core capabilities:

- Chemicals: Council for Chemical Research
- Refining: American Petroleum Institute
- Forest products: American Forest and Paper Association
- Steel: American Iron and Steel Institute
- Aluminum: Aluminum Association, SECAT LLC
- Metal casting: Cast Metal Coalition
- Glass: Glass Manufacturers Industry Council

In other work, one of our initiatives aims to develop less costly biotechnological methods of producing valuable products from agricultural materials. See the discussion of Biobased Products in Section IV.A.2.f.

Superconductivity. There is increasing conviction among electric utilities and their suppliers that new technology based on high-temperature superconductivity will provide substantial benefits. This industry support is reflected in projected increases in DOE funding of R&D in the area. Several respected international studies have predicted that global annual sales for all technologies based on high-temperature superconductivity will reach billions of dollars by the year 2020. International competition for these sales will be strong, particularly from Japan and Western Europe.

Argonne is uniquely positioned to develop new technologies based on high-temperature superconductivity. Our program of basic science in the field is one of the strongest in the world. Close cooperation continues with the Laboratory's applied superconductivity program, which has produced many notable achievements. We plan to be a major contributor to the development of the second-generation conductor, building on industrial successes already achieved with first-generation powder-in-tube technology. We also are contributing to the development of a flywheel incorporating superconducting bearings. We will expand the range of utility applications on which we work, particularly by taking advantage of new ideas for fault-current limiters, transmission cables, and motors based on superconductivity. Work in nonutility applications will expand as well, on the basis of innovative ideas in areas such as magnetic separation.

Fossil Fuels and Carbon Management. Support for DOE research related to carbon management is growing. A consortium of major petroleum companies is working with the DOE Office of Fossil Energy to plan field demonstrations of technologies for the economical sequestration of carbon dioxide. The President's FY 2004 budget request includes additional funding for R&D in this area and for regional sequestration initiatives.

Partnering. Congressional appropriations have continued to reduce funding explicitly available for participation by DOE in industrial partnerships. Our industrial partnerships have been severely constrained by this lack of support. The President's FY 2004 budget request includes termination of the multilaboratory partnership in oil and gas exploration and development.

To maximize the likelihood of establishing effective industrial partnerships in the most promising areas of technology, we seek opportunities to include other national laboratories and universities in productive strategic collaborations based on our scientific and technical capabilities and our core competencies. We have already established a vigorous regional outreach program whose broad goal is to help manufacturers in the Midwest. We measure the success of our industrial partnerships by considering the significance and impact of the work accomplished and of the ultimate successful commercialization of new technologies.

c. Transportation Technologies

Situation

The world's transportation system depends critically on petroleum. Oil-derived fuels supply 96% of the energy used to move people and goods. Demand for these fuels continues to grow rapidly, rising by 75% in the United States since the oil crises of the 1970s. Worldwide, the demand for transportation fuels is expected to increase dramatically, especially as developing economies grow. As a result, the world is rapidly approaching the time when a permanent decline in oil production from conventional sources will begin. The Energy Information Administration forecasts that conventional oil production could begin to decline between 2010 and 2040. As the relative price of transportation fuels rises, vehicles with greater energy efficiency will become increasingly important.

Two major research programs led by DOE are designed to reduce oil demand by developing vehicles with greater energy efficiency. These programs are the FreedomCAR and Fuel Initiative (for light-duty vehicles) and the 21st Century Truck Program (for heavy-duty vehicles). Successful development of vehicles that are dramatically more efficient, along with development of alternative fuels, would reduce oil imports, increase energy security, and reduce environmental impacts.

Our Transportation Technology R&D Center is one of DOE's leading research facilities dedicated to addressing the nation's transportation energy problems. Located in the heart of the Midwest, near the nation's manufacturers of automobiles, trucks, and locomotives, we work closely with both manufacturers and suppliers to develop cost-effective technologies that improve fuel efficiency and reduce environmental impacts. As part of this effort, we maintain a web site that describes the research facilities and capabilities of our Transportation Technologies program (URL: www.transportation.anl.gov).

Vision

Transportation and energy infrastructure will always be critical to U.S. national security. Our Transportation Technology R&D Center will become the premiere provider of needed knowledge about advanced transportation technology and its application, for the nation's industrial, academic, and government research communities.

Goals and Objectives

Our Transportation Technology R&D Center will support the nation's needs for R&D on transportation technology. This goal will be accomplished through basic research, through technology development, and through the creation of partnerships with industry, academia, and other federal or national laboratories that promote energy self-sufficiency and improve energy- and transportation-related technologies serving the national interest.

Specific objectives include the following:

- Work with the FreedomCAR program and Fuel Initiative (spearheaded by the DOE Office of Energy Efficiency and Renewable Energy, in partnership with Ford, General Motors, and DaimlerChrysler) to
  - Ensure reliable systems for future fuel cell powertrains, with costs comparable to those of conventional systems (internal combustion engine with automatic transmission) and

- Enable the transition to a hydrogen economy, ensure widespread availability of hydrogen fuels, and retain the functional characteristics of current vehicles. (See the major Laboratory initiative Hydrogen Research and Development in Section III.B.2.)

• Work with DOE and truck engine manufacturers to improve the efficiency and reduce the emissions of advanced diesel technology for use in vehicles of all sizes, as well as to assess the health risks associated with different fuels and engines.

• Develop new technology with a private-sector partner — General Motors Electro-Motive Division — to meet federal locomotive emissions requirements and still achieve high efficiency.

• Work with DOE to develop advanced off-highway and railroad technologies, on the basis of opportunities identified in consultation with industry stakeholders.

Issues and Strategies

Our transportation research, domestic and international, focuses on the following areas where we have recognized expertise and unique facilities:

• *Vehicle Systems*. New vehicle systems promise to overcome the main limitations of conventional electric vehicles, namely range and recharging rate. Hybrid vehicles typically employ a small combustion engine with a battery or ultracapacitor. The result is the performance of a conventional vehicle but greater efficiency and decreased emissions. Our Advanced Powertrain Research Facility validates DOE-funded components with data on performance and emissions. The Laboratory's vehicle systems models can then simulate actual vehicle systems performance and emissions.

• *Fuel Cells*. Fuel cells convert chemical energy directly into electrical energy, cleanly and efficiently. Fuel-cell-powered vehicles could nearly double the energy efficiency of today's conventional vehicles and reduce emissions by 99%. We have developed a partial-oxidation reformer that converts gasoline to hydrogen-rich gas for use in fuel cells based on polymer electrolyte membranes. Our Fuel Cell Test Facility is capable of testing fuel cells up to 50 kW in size. We are also developing solid oxide fuel cells for transportation use.

• *Energy Storage Devices*. In response to stringent environmental regulations, we are developing advanced batteries for electric vehicles. In particular, we are working through the U.S. Advanced Battery Consortium to develop commercially viable high-power lithium-ion storage batteries. This work ranges from research on materials for improved anodes and cathodes to development of novel, low-cost packaging. Our Battery Test Facility performs independent evaluations of batteries developed worldwide.

• *Emissions Control*. By focusing on fuel injector systems and sensors, we plan to develop technologies that simultaneously reduce emissions of particulates and nitrogen oxides from gasoline and diesel engines of all sizes. Until recently, the optically dense regions of the fuel spray from injector systems have been very difficult to image. However, insights gained by using the world's brightest x-rays, provided by the APS, promise improved understanding of combustion and soot formation, leading to the development of cleaner and more efficient engines.

• *High-Performance Computing*. We have supported the transportation industry in the design and testing of new concepts for aerodynamics, thermal management, and safety features. Major efforts in this area involve analyzing underhood cooling and crashworthiness.

• *Recycling*. Obsolete motor vehicles contain plastics, chlorofluorocarbons, rubber, glass, and heavy metals that today are generally not recyclable and must be put into a landfill. Working closely with the auto industry, we are developing economical processes for converting vehicle waste streams into recycled products.

• *Advanced Materials*. Our advanced materials program includes the development of nearly frictionless carbon coatings to reduce the friction and wear caused by sliding and rotating vehicle components. The program also includes the development of new technologies for sensors, rapid prototyping, nondestructive evaluation of ceramic parts, compact heat exchangers, and nanofluids for coolants. Each of these materials technologies promises to improve both the performance and fuel efficiency of vehicles. Use of the APS is expected to assist in the development of catalysts and other new transportation materials.

d. Environmental Treatment Technologies

Separate plans are presented below for three areas of environmental treatment technologies at Argonne: (1) EBR-II spent fuel pyroprocessing, (2) radioactive and mixed waste treatment, and (3) decontamination and decommissioning (D&D).

i. EBR-II Spent Fuel Pyroprocessing

Situation

For nearly four decades, research, development, and demonstration associated with liquid metal fast breeder reactors were conducted at EBR-II, located about 40 miles west of Idaho Falls, Idaho; the Enrico Fermi Atomic Power Plant (Fermi-1) in Monroe, Michigan; and the Fast Flux Test Facility at the Hanford Site in Richland, Washington. These activities generated approximately 60 metric tons of sodium-bonded spent nuclear fuel. DOE is now responsible for safe management and disposition of this spent fuel.

Sodium-bonded spent nuclear fuel must be treated differently from other spent fuel because of the presence of metallic sodium (a highly reactive material), metallic uranium and plutonium (also potentially reactive), and, in some cases, highly enriched uranium. Metallic sodium in particular presents challenges for the management and ultimate disposal of spent nuclear fuel, because the element reacts with water to produce explosive hydrogen gas, as well as corrosive sodium hydroxide that is likely to be unacceptable for geologic disposal.

Argonne’s pyroprocess for treating metallic spent nuclear fuel uses electrorefining, a type of technology often used by industry to produce pure metals from impure feedstocks. Application of our pyroprocess has been demonstrated for the stainless-steel-clad uranium alloy fuel and blanket assemblies from EBR-II. A modified process could be used to treat oxide, nitride, and carbide sodium-bonded spent nuclear fuel.

Application of pyroprocessing to EBR-II spent fuel involves several steps. The fuel is first chopped, placed in molten salt, and electrorefined. After electrorefining, the molten salt, fission products, sodium, and transuranics (including plutonium) are removed from the electrorefiner, mixed with the ion exchange agent zeolite, and heated so that the salt becomes sorbed into the zeolite structure. Glass powder is then added to the zeolite mixture and consolidated to produce high-level radioactive waste in the form of a ceramic. The uranium from the electrorefiner is removed, melted, and processed in a furnace to produce low-enrichment or depleted uranium ingots. The stainless steel cladding hulls and the insoluble fission products are melted in a casting furnace to produce high-level radioactive waste in metallic form.

A three-year demonstration of treating EBR-II spent nuclear fuel was completed in 1999. A subcommittee of the National Research Council judged that the demonstration met all success criteria. DOE then selected pyroprocessing (also known as electrometallurgical treatment) for the complete inventory of EBR-II sodium-bonded fuel, work now under way at Argonne-West.

Vision

Through treatment of EBR-II and other sodium-bonded spent fuel, we will demonstrate that pyroprocessing technology is a cost-effective option that provides a viable approach to managing spent nuclear fuel.

Issues and Strategies

In September 2000 we initiated treatment operations with EBR-II fuel. Processing rates were increased from the demonstration rates to a total of 600 kilograms per year. As funding becomes available for additional staffing and technology advancement, the processing goal for the following year will be increased. The capacity rate of 5 metric tons per year is to be reached after processing improvements are implemented and staffing is increased.

An important issue associated with treatment of EBR-II spent fuel is continued development of the pyroprocess treatment technology in order to achieve the throughput rates required for economical operation. Although the basic technology has been demonstrated, product losses and waste streams should be reduced, new equipment should be produced, and batch size should be optimized. The cost of continued technology development will be a significant fraction of total costs during the first several years of operation.

Waste form development and qualification will extend well into the schedule for treating EBR-II spent fuel, because licensing of the new waste forms for ultimate disposal in a repository requires completion of an extensive behavior characterization database, reflecting both short-term tests and long-term tests with actual radioactive wastes that will extend several more years. Nevertheless, tests with surrogate fission products and limited tests with actual radioactive waste forms have provided sufficient data to establish the viability of the new waste forms.

ii. Radioactive and Mixed Waste Treatment

Situation

Many of DOE's highest-priority business goals depend directly on the Department's environmental program, specifically on the objectives of the DOE Office of Environmental Management (DOE-EM). Included in the DOE-EM plan is application of new technologies that have reached various stages of development with support from the DOE-EM Office of Science and Technology.

We have demonstrated significant core capabilities in advanced environmental technologies, built on our broad competencies in nuclear technology and environmental science and technology; our existing nuclear facilities; and our extensive understanding of — and experience in resolving — complex environmental problems at sites of DOE, Department of Defense (DOD), other federal agencies, and U.S. industry. Integration of capabilities in environmental research, technology development and deployment, comprehensive assessment, and remediation applications is the basis for our continuing development of advanced environmental technologies tailored specifically to particular facilities and waste streams for many different types of customers.

To support DOE's Central Characterization Program, Argonne-West will perform solid core sampling of contact-handled transuranic materials (homogeneous solids or soils and gravels). Beginning in the spring of 2003, this work is being done in the Waste Characterization Area of the Hot Fuel Examination Facility (HFEF). In the DOE complex, about 700 drums are estimated to require core sampling. The work will be completed in approximately five years.

We plan to construct the Remote Treatment Facility (RTF) at Argonne-West to provide the infrastructure needed to carry out three missions important to DOE, the state of Idaho, and the national nuclear complex: (1) near-term management of wastes resulting from nuclear research conducted in earlier years at Argonne-West and INEEL, (2) R&D to achieve nuclear energy and national security goals, and (3) R&D to achieve environmental technology goals. Special needs in each of these three areas require that DOE operate facilities dedicated to the development, testing, and implementation of technologies and processes involving the remote handling of highly radioactive materials and the use of intense radiation sources. We will operate the RTF both to meet local waste management needs and to serve as a national user facility for the development and testing of remote technologies. The RTF will augment the existing HFEF at Argonne-West. Development of the RTF will include an addition to the present HFEF and integration of existing HFEF support capabilities, such as analytic chemistry laboratories, into RTF operations.

The mission need for the RTF has been confirmed by DOE-NE. As a result, inclusion of funding for RTF design and construction is expected in DOE's FY 2005 budget request.

Vision

We will advance understanding of environmental problems and will develop technologies that allow cost-effective remediation or prevention of those problems for nuclear waste, mixed waste, and other contaminants.

Objectives

Our work on advanced environmental technologies has the following central objectives:

- Develop technologies and facilities for treating mixed waste and nuclear materials.
- Develop superior waste forms and methods of testing and validating techniques for predicting performance.
- Develop innovative environmental technologies that exploit the state of the art in separation science, chemical interactions, and advanced materials.
- Integrate scientific research with field engineering experience and methodologies in order to develop cost-effective solutions to environmental problems.

These Argonne objectives clearly help to address the following two "gaps" identified in DOE's September 2000 R&D portfolio analysis for its Environmental Quality mission area: (1) dispose of transuranic, low-level, mixed low-level, and hazardous waste (gap number 8) and (2) manage nuclear material (gap number 6).

Issues and Strategies

Development of advanced technologies for mixed waste treatment is a logical extension of our broad background in reactor technology. In mixed waste treatment, we plan to continue to specialize in remote-handling operations, transuranics, waste form development, environmental process monitoring, and nonthermal treatment options.

Argonne-West already deals with significant amounts of remotely handled radioactive and mixed wastes, which are stored at its Radioactive Scrap and Waste Facility. These wastes require additional characterization, segregation, treatment, and repackaging.

The RTF will be designed to segregate, characterize, treat, and repackage remotely handled materials. The essential features of the RTF are an air atmosphere hot cell with 13 workstations, a hot repair area with access to the hot cell, waste cask handling capabilities, and a cell for nondestructive analysis. Equipment to be installed in the RTF includes a liner disassembly station, an automated waste sorting station, a sodium removal station, an induction furnace, and a waste repackaging station. Direct linkage with the HFEF will be through a cask tunnel. The cask transfer system will be capable of dealing with many types of casks, including the commercial nuclear fuel casks that are licensed for remotely handled transuranic waste. Waste packages that are not compatible with casks will enter the RTF cell through the hot repair area.

Development of stabilized waste forms is very important for solving problems associated with high-level and mixed waste. During the last decade, we have performed a wide range of R&D contributing to waste form development, including long-term and accelerated testing of high-level waste glasses and technical support to the Yucca Mountain Project, development of room-temperature setting of chemically bonded phosphate ceramic waste forms, studies of glass compositional envelopes for DOE-EM, definition of performance specifications for Hanford low-level wastes, and phosphate mineralization of actinides achieved by the measured addition of precipitating anions. We will continue to support DOE programs such as the high-level waste repository and the Waste Isolation Pilot Plant. In addition, technical support will be provided to DOE field offices and to the site contractors at major sites charged with cleanup and waste management, such as Savannah River, Fernald, Rocky Flats, INEEL, and Hanford.

We will continue to support DOE-EM R&D aimed at long-term disposal of waste forms. This research centers around the physics and chemistry of surfaces and interfaces; development of new waste forms for "problem" wastes; and modeling, validation, and performance testing.

iii. D&D

Situation

Decontamination and decommissioning of production and research reactors and nuclear manufacturing facilities represents a major challenge for DOE and the commercial nuclear industry. Problems associated with D&D include safe and effective dismantlement of contaminated and radioactive components; packaging, transportation, and disposal of waste; and recycling and reuse of material.

We are uniquely positioned to assume a leadership role in the development and demonstration of D&D technologies. A number of the technologies already developed or under development at Argonne can be applied to D&D, including advanced cutting technologies (such as lasers, water jets, and plasma arcs), telerobotic systems, effluent control technologies (such as filters for aerosols and dissolved contaminants), instrumentation, decontamination methods (both chemical and mechanical), and risk assessment methods.

We are building our D&D technology program on a strong foundation of extensive experience in nuclear and environmental work, recent success in applying D&D technologies, and valuable strategic partnerships. We have experience with the D&D of many types of nuclear facilities, including reactors, hot cells, and facilities containing glove boxes. The most significant of our reactor D&D projects involved the CP-5 Research Reactor and the Experimental Boiling Water Reactor. We also have a long history of developing and deploying both nuclear and nonnuclear technologies, and we have played a leading role in this country's first D&D technology demonstration program at a working D&D site. The CP-5 Large Scale Demonstration and Deployment Project was judged one of DOE's "Top 100 Achievements of the Century." We have been instrumental in developing risk-based analyses for recycle and release criteria and for transportation. Our RESRAD (RESidual RADioactivity) family of computer codes is widely used by regulators to aid in evaluating compliance, through estimation of doses and related risks to human health and the environment that result from exposure to radioactivity and chemically contaminated materials. We have also developed cost engineering models that have been used to validate cost estimates throughout the DOE complex. We are active in several international organizations involved in D&D and have initiated information exchange programs with the IAEA, Japan, Russia, and Argentina.

Vision

To optimize the cost-effectiveness and safety of D&D operations, our D&D technology program will continue to advance the development, demonstration, and deployment of cost-saving D&D technologies and to develop and execute analyses of risk, safety, environmental impacts, and costs for DOE, other federal agencies, regulators, and the commercial sector. The program will also continue its contributions to D&D education through training, workshops, and personnel exchanges.

Objectives

The main objectives of our D&D technology program are the following:

- Provide substantive information on the use and value of D&D technologies for all categories of end users.
- Coordinate the research, development, demonstration, and evaluation of D&D technologies in order to achieve cost-effective D&D for the DOE complex.
- Provide technical services and support in the areas of risk, safety, and cost analysis, as well as in planning and technology deployment.
- Provide D&D training and participate in informational and educational exchange both domestically and internationally, including support for D&D in the former Soviet Union.
- Work with the DOE Environmental Management Science Program to encourage basic research in areas that will benefit D&D technology.

Issues and Strategies

Key to the development of our D&D technology program is formation of strategic alliances among national laboratories, utilities, universities, D&D contractors, and technology developers and providers. We will continue to pursue appropriate alliances with nuclear utilities and D&D contractors, as well as with the Nuclear Energy Institute and the Electric Power Research Institute. In all our D&D technology efforts, we work closely with DOE-Chicago Operations. Internationally, we will take advantage of our strong international research reactor program, which dates back to Argonne's design of research reactors and, more recently, to the design and implementation of proliferation-resistant fuels for research reactors.

A number of external and internal factors will influence the success of our D&D technology program. External factors include scheduling of D&D by DOE and utilities, effects of utility deregulation, and the availability of low-cost disposal sites for low-level nuclear waste. Internal factors include close integration of our diverse capabilities in technology and advanced technical services. Equally important is the formation of partnerships and strategic alliances with organizations outside the Laboratory.

e. Energy and Environmental Systems

Situation

Long-term energy resources and environmental impacts from energy consumption remain controversial public concerns complicated by economic importance and contradictory public perceptions. Informed decision making in this area requires accurate, clearly presented analyses based on a very wide range of technical information. Federal policy analysis is further complicated because responsibilities relating to energy and the environment are spread widely across federal agencies. No single agency has a mandate to examine the full range of relevant issues.

For decades, we have created technically and economically efficient solutions for energy and environmental problems by applying scientific methods in the development and assessment of new and modified technologies and processes. Our successes in this area stem from our capacity to assemble interdisciplinary teams of specialists and to integrate diverse technical resources in order to address difficult problems through focused study and exploitation of unique facilities. A particular Argonne strength is our capability for merging decision analysis, risk assessment, information sciences, and economic evaluations with the engineering specialties and the physical, biological, and social sciences.

Energy and environmental problems create these challenging national needs:

- The rapidly growing complexity of the energy system and related environmental issues such as water resources necessitate a multidisciplinary, integrated approach to solutions.
- Solutions to environmental problems must be both cost-effective and acceptable to the public.
- The growing information glut facing all decision makers requires the development of better ways to capture, merge, and display critical information.
- Such policy areas as climate change, pollution remediation, and resource management increasingly require global analysis and international coordination.
- There is growing evidence that restructuring of the U.S. electric system requires new approaches to reliability, environmental protection, and preparation for disruptions. At the same time, new environmental regulations require the development and adoption of advanced procedures and technologies.
- The benefits of increasing the production of fossil fuels on U.S. public and private lands must be balanced against the need to protect environmental quality.
- Analysis of hydrogen as a basis for future energy systems will require a highly multidisciplinary approach. (See the major Laboratory initiative Hydrogen Research and Development in Section III.B.2.)

Vision

Argonne will provide national and international leadership in the creation of innovative and cost-effective solutions to energy and environmental problems, through the development of next-generation technologies; through the application of state-of-the-art techniques in assessment, risk analysis, and decision analysis; and through the transfer of those technologies to the private sector and other researchers.

Objectives

Key objectives of our program in Energy and Environmental Systems include the following:

- In order to improve the analysis and assessment of advanced energy systems, develop models, methodologies, and techniques that give decision makers more accurate information about the changing structure of the energy system.
- Develop integrated environmental assessments, risk analyses, modeling techniques, and innovative information systems — by using approaches such as advanced visualization, advanced data management techniques, and spatial and geographic information systems — that benefit federal managers, policy makers, and private-sector businesses facing new regulatory requirements.
- Apply these energy and environmental tools, techniques, and methodologies to issues of national concern; transfer the tools to other researchers and to private-sector energy organizations for improved decision making.
- To improve the cleanup and subsequent long-term stewardship of Cold War legacy waste sites, make available more widely — to DOE, federal, and private-sector sites — the benefits of Argonne's unique capabilities in information management; in tools for assessing the changing structure of energy systems; and in methods of site characterization, remediation, and restoration.
- Expand our international activities that address global climate change and environmental protection.

Issues and Strategies

Our strategies for achieving our objectives in Energy and Environmental Systems include the following:

- Take advantage of Argonne's strengths in high-performance computing and multidisciplinary domains to investigate the application of advanced techniques — such as complex adaptive systems analysis and agent-based simulation — and provide better decision making information in the rapidly changing, highly complex, nonlinear arena of energy and environmental policy.
- Combine innovative decision tools with field techniques to create applied environmental methodologies that are more effective. For example, tailor more cost-effective approaches to site cleanup and long-term stewardship through better site sampling strategies, better monitoring methodologies, and more flexible decision-making practices based on rapid acquisition and evaluation of accurate field data.
- Address emerging technical issues associated with long-term environmental stewardship at DOE and other federal facilities, especially sites requiring extensive cleanup. (See discussion of the initiative Science and Technology for Environmental Stewardship at the end of this area plan.)
- Collaborate with urban community groups to increase the stock of energy-efficient buildings, including housing and schools; to return abandoned sites to use; and to design and implement next-generation modes of urban transportation. These efforts will include integration of Argonne techniques, technologies, tools, and training to foster the creation of more high-wage jobs, to ease urban blight, and to support the renovation of urban infrastructure.
- Explore additional opportunities to apply our special capabilities beyond DOE, to benefit the Departments of Defense, Agriculture, and the Interior; the Nuclear Regulatory Commission; other federal agencies; state and municipal governments; nongovernmental organizations; and the private sector.

• With international organizations and appropriate foreign governmental organizations, expand activities involving the analysis of international issues concerning energy and environmental systems — including global electric system restructuring, transnational energy system interconnections, global climate change, sustainable development, hazardous waste generation, and ecosystem management.

In summary, we have considerable strength in most scientific and technical areas related to energy and the environment. We are well organized to integrate our multidisciplinary capabilities in research, development, and demonstration of new technologies. Recognition of these capabilities has allowed us to develop solutions to a wide variety of real-world problems and to further strengthen our relationships with sponsors. Current challenges include developing innovative methodologies for analyzing energy and environmental problems (such as global climate change, restructuring of the electricity market, and the hydrogen economy) that cannot be addressed adequately with conventional techniques; identifying appropriate opportunities for beneficial external collaboration; and extending the breadth and depth of the Laboratory's capabilities.

Initiative: Science and Technology for Environmental Stewardship

The DOE R&D portfolio analysis for the Environmental Quality mission area in September 2000 identified long-term environmental stewardship as one of four highest-priority technical "gap" categories. In response to this need, we propose a program of research, development, and analysis to address emerging technical issues associated with the environmental stewardship of lands and facilities for which DOE and other federal agencies are responsible.

The concept of environmental stewardship encompasses the mechanisms — physical and institutional controls, information management, environmental monitoring, risk assessment, and other means — needed to ensure, in both the short term and the long term, protection of people and the environment. Government is responsible for stewardship of the lands it manages and for the environmental consequences of its activities. Planning for effective stewardship includes evaluating impacts from the use of rights-of-way on federal lands (such as the Trans-Alaska Pipeline system); assessing the effects of extracting energy and other resources; and developing effective methods of managing residual contamination left following cleanups at government facilities.

This initiative in Science and Technology for Environmental Stewardship takes advantage of our substantial capabilities and experience in characterization, in analysis and engineering for processes and systems, and in integrated management, including risk assessment. The initiative will emphasize (1) decision making related to risk to human health and ecosystems and (2) monitoring to obtain feedback for updating previous decisions. Such risk assessment requires integration of results from multiple analyses, models, and monitoring. Associated decision making processes often involve disparate stewards, regulators, and the public. Informed decision making depends critically on effective integration and dissemination of relevant information. To create an improved technical basis for stewardship, we will investigate the deployment of technologies and approaches we have developed by using advanced techniques of computing and communications.

Resources that can be applied beneficially to this initiative are described in Table IV.5. Funding will be sought initially from DOE-EM (EW, EX); DOE-Environment, Safety and Health (HC); DOE-Science (KP-12, KP-13); and the new DOE Office of Legacy Management.

Table IV.5 Science and Technology for Environmental Stewardship ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	9.7	10.0	13.0	15.0	17.0	19.0	19.5
Capital Equipment	0.3	0.4	0.5	0.5	0.5	0.5	0.5
Construction	-	-	-	-	-	-	-
Total	10.0	10.4	13.5	15.5	17.5	19.5	20.0
Direct Personnel	30.0	32.0	39.0	40.0	41.0	42.0	43.0

f. Biotechnology

Situation

Biotechnology research at Argonne is a multidisciplinary, cross-cutting activity that integrates a variety of disciplines and unique research facilities. We are one of DOE's leading resources for developing the technologies of biological microchips and biobased chemicals. Key elements of our program are sponsored by DOE, DOD, and private-sector industrial collaborators. Near-term plans include further strengthening of capabilities in biocatalytic and downstream processing, in bioinformatics, and in the development of automated systems for gene cloning and expression.

Objectives

Key objectives of our biotechnology program include the following:

- Develop integrated systems for the automated acquisition and processing of environmental samples and the use of downstream detection (e.g., biochips) for analyzing complex samples.
- Evaluate biochemicals for control of cellular malignancies.
- Develop advanced emergency resuscitation technologies, improved artificial intelligence for medical diagnostics, and new prosthetic materials and coatings.
- Develop environmentally advantageous bioprocessing technologies (notably integrated biocatalysis and separations) for application to biological and chemical feedstocks.
- Develop technologies to monitor, remove, detoxify, and recover heavy metals, organic compounds, and bacteria in the environment.

Issues and Strategies

In addition to national security, our programs in biotechnology focus on three promising areas having high national priority:

- *Medical Applications.* Programs emphasize development of advanced biochips for analyzing genetic information, studying cancer and biochemicals to guide pharmaceutical development, and developing advanced devices and procedures for emergency resuscitation.
- *Industrial Processes*. Programs include the development of separations and their integration with biocatalysis to produce environmentally advantageous products (e.g., polymer-grade monomers and "green" solvents such as succinic acid, acetic acid, lactic acid, and ethyl lactate) through bioprocessing of chemical feedstocks (e.g., syngas) or biobased feedstocks (e.g., lignocellulose or corn). Also considered are biobased batteries and biohydrogen production in new types of separative bioreactors.
- *Environmental Protection.* Programs include investigation of environmentally acceptable methods for treating microbial corrosion in pipelines; field demonstrations of phytoremediation methods; and development of photocatalysts for the removal, detoxification, and recovery of heavy metals and organic compounds in aqueous waste streams. We are also developing, with former weapons scientists from the former Soviet Union and U.S. partner companies, nonproliferation programs in areas such as biocorrosion and phytoremediation.

Initiative: Integrated Biodetection Systems

Our established biochip program is invigorated by the development of both defense and nondefense applications that use biochips to detect nucleic acids, peptides, and proteins. Current spinoff initiatives focus on five key areas:

- Integrated biodetection systems
- Nucleic acid chips
- Protein chips
- Polymerase chain reaction (PCR) chips
- Metabolic chips

Our patent portfolio covers three-dimensional biochips and associated technologies. This gel pad configuration allows each pad to function as a test tube for protein reactions, PCR, and other processes. Our biochip program is closely linked to our biodefense work for DOD and NIH and to work for DOE's Genomes to Life program, as well as to work on environmental applications and biomedical diagnostics. Resources required for this initiative are summarized in Table IV.6. The funding increase for FY 2004 is sought from DOE, other federal agencies, and the private sector.

Table IV.6 Integrated Biodetection Systems ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	2.4	3.0	3.5	3.5	3.5	3.5	3.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	2.4	3.0	3.5	3.5	3.5	3.5	3.5
Direct Personnel	6.0	6.5	7.0	7.0	7.0	7.0	7.0

Initiative: Biobased Products

Our biobased products program, like our biochip technology program, is an established activity that often spins off initiatives as novel potential applications are identified. Current components of the Biobased Products initiative range from the development of additional uses for corn as a chemical feedstock to the development of advanced membrane processes that lower the cost of downstream processing and purification. We are also developing a separative bioreactor that could transform separations for organic acids and other chemicals from the current costly multi-step process to a single efficient step. Nanoscience and structural biology are being applied to address fundamental issues in biocatalysis and processing, particularly issues that affect product cost. Resources required for this initiative are summarized in Table IV.7. Funding is sought from DOE-Energy Efficiency and Renewable Energy (ED), DOE-Fossil Energy (AA), other federal agencies, and industrial partners.

3. National Security

As stated by Secretary Abraham, national security is the overarching mission of DOE. It is also one of the four traditional underlying mission areas of the Department.

Table IV.7 Biobased Products ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	1.5	1.5	1.5	1.5	1.5	1.5	1.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	1.5	1.5	1.5	1.5	1.5	1.5	1.5
Direct Personnel	4.0	4.0	4.0	4.0	4.0	4.0	4.0

a. Nuclear National Security

Situation

Our current work on nuclear national security aims to reduce threats posed by nuclear and radiological materials. At the end of the Cold War, the principal threat to U.S. national security changed from large-scale nuclear war to asymmetric conflicts and terrorism by subnational groups. Our earlier focus on technical means of verifying treaty compliance has shifted toward developing ways to limit the spread of weapons of mass destruction and also radiological weapons that can cause widespread disruption and impose large costs.

Among the most pressing problems facing the United States is the breakdown of systems for controlling nuclear materials in Russia and the independent states that resulted from the dissolution of the former Soviet Union (FSU). The United States, with several other countries, is providing technical assistance to help FSU nations improve their control systems. A further major concern is radiological materials located throughout the world, for which only limited controls are now in place. In this case as well, the United States is one of several countries providing technical assistance to improve security and controls.

Our nuclear national security program, with an annual budget totaling approximately $20 million, includes several significant components:

- The Reduced Enrichment for Research and Test Reactors (RERTR) program, which develops new fuels, targets, and analysis methods to enable research reactors throughout the world to substitute low-enrichment uranium for the highly enriched uranium in their fuel and targets.

• The Material Protection Control and Accounting (MPC&A) program, which assists nuclear facilities in Russia and the independent FSU countries. Assistance is offered through surveying the current status of protection and accounting for nuclear materials, making recommendations for improvements, and coordinating upgrade plans and their implementation. This program includes training courses, offered both at Argonne and abroad, that enable foreign specialists to effectively utilize new security and accounting systems.

• The Verification Technology program, which develops sensitive and selective instruments to detect radiation and chemical and biological effluents that might indicate clandestine proliferation.

• The Nuclear Export Control program, which provides technical assistance to the National Nuclear Security Administration (NNSA). This assistance includes (1) assessments of proliferation risk associated with proposed exports of nuclear and nuclear-related dual-use material, equipment, and technologies and (2) establishment and improvement of effective systems of export control in the independent FSU countries, supplier countries, and countries through which relevant materials and equipment are transported.

• Transportation and final storage of nuclear materials from the BN-350 breeder reactor in Kazakhstan, which implements U.S. non-proliferation goals by improving the security of the plutonium from the reactor's spent fuel and blanket assemblies.

• Irreversible shutdown of the BN-350 breeder reactor, which serves U.S. nonproliferation goals by ensuring that the reactor can never again produce nuclear materials suitable for weapons. This program utilizes a unique organizational approach in which integrated design teams are established between various Kazakhstan organizations and Argonne in order to resolve issues that arise.

• The joint U.S.-Russian materials disposition program, which targets the disposal of excess weapons plutonium by reactor irradiation. As part of this effort, the BN-600 fast reactor is being converted to a configuration that burns plutonium.

• The Highly Enriched Uranium Transparency program, which monitors the blending down of highly enriched uranium from dismantled Russian nuclear weapons to produce low-enrichment uranium for eventual use as commercial reactor fuel in the United States, thereby encouraging compliance with international treaty obligations and reducing the threat of nuclear proliferation.

• The Initiatives for Proliferation Prevention (IPP) and the Nuclear Cities Initiative (NCI), which engage former nuclear, biological, and chemical weapons workers in Russia, Ukraine, and Kazakhstan in developing peaceful new civilian occupations. This effort involves collaboration with U.S. companies working under cooperative R&D agreements with Argonne scientists. (The NCI helps only workers in Russian closed cities.)

• The Radiological Dispersal Device program, which helps to secure the radiological materials located abroad that pose the greatest risk to U.S. security, though visits by technical assessment teams comprising experts in physical security, materials control and accounting, and health physics.

Mission

By exploiting the technical and analytical expertise of our staff and our facilities for nuclear research, we support the efforts of federal agencies to reduce threats to national security resulting from the proliferation or possible use of weapons of mass destruction and radiological weapons capable of causing mass disruption. In addition, we help to implement associated U.S. policy initiatives.

Issues and Strategies

We plan to integrate and increase our support for nuclear national security initiatives, particularly by exploiting our unique expertise in nuclear and sensor technologies. The RERTR activities will involve extensive cooperation with Russia and more than 25 other countries. Many international research reactors are today fueled with highly enriched uranium and cannot be converted to low-enrichment fuel by using current technologies. We plan to develop the required new nuclear fuels. In addition, we will develop new targets and chemical processing to produce molybdenum-99, an important medical radio-isotope, by using low-enrichment uranium instead of highly enriched uranium. Our expertise will be used to enhance the security of nuclear materials at additional sites in the FSU and also to reduce the availability of weapons-usable materials by reducing stockpiles of highly enriched uranium. Other activities will focus on developing spin-off projects related to our established MPC&A and training programs in Russia and independent FSU countries. Our technical staff will continue to support NNSA efforts to promote effective nuclear export controls. Argonne expertise will also assist in the development of radiological materials detectors. The IPP program will be extended to engage former biological and chemical weapons workers in the FSU. The NCI program will help place former nuclear weapons scientists in commercial projects at the Sarov Open Computing Center. On the basis of our expertise in nuclear fuel management, we have a technical leadership role in the final storage of the spent nuclear fuel at the BN-350 fast reactor in ways that improve resistance to proliferation. In addition, we were selected to serve as one of two lead laboratories for a proposed project to assist Russia with the design and construction of a dry storage facility for fuel awaiting reprocessing at Mayak. The initiative Nonproliferation Technologies, discussed below, proposes significant expansion of our work on the development, demonstration, and deployment of nuclear material safeguard technologies.

Recent terrorist attacks have made clear the need for increased attention to nuclear national security and homeland defense. Weapons of mass destruction and the materials that are key to their production must continue to receive intense attention. Moreover, the need to address nontraditional challenges, such as weapons that can cause massive disruption, has risen to unprecedented importance. Systems originally designed to address more traditional threats must evolve in order to plan adequately for new potential targets, different modes of delivery, different weapons, and different consequences, including functional defeat of critical economic infrastructure and processes. Systems for responding to actual events must also evolve.

To reduce threats from domestic and international nuclear events, we propose five new initiatives:

1. Nonproliferation Technologies
2. Nuclear Fuel Cycle Technology Applications
3. Training for Specialists in Nuclear Material Protection and Law Enforcement
4. International Nuclear Safety and Cooperation
5. Integrated Research Reactor Safety Enhancement Program

Initiative: Nonproliferation Technologies

We propose significant expansion of our activities related to the development, demonstration, and deployment of nuclear material safeguard and process monitoring technology. For NNSA and DOE-EM, our established sponsors in these areas, this initiative addresses nondestructive assay of materials, monitoring and surveillance systems, and advanced software products. We will also leverage our expertise in special nuclear material handling and physics, along with our associated facilities and materials, to conduct process testing of related technologies developed at Argonne and elsewhere in the DOE complex. Technology development initiatives will be tied to our unique physical resources — including our nuclear materials and remote handling facilities — and ongoing nuclear technology projects. These broadly applicable technologies could also serve DOE-Civilian Radioactive Waste Management and DOD, as well as other federal agencies. As part of this initiative, we also propose to help develop detectors for discerning the movement of radiological dispersion devices and to assist training on the threats these devices pose.

This Nonproliferation Technologies initiative strongly leverages core Argonne programs in spent nuclear fuel treatment, nuclear waste, nonproliferation, facility operations, nuclear safety modeling, and other areas. Related work supporting the Office of Emergency Response of the NNSA aims at technical integration to produce deployable tools and technologies for responding to nuclear and radiological emergencies.

Funding for this initiative will be sought from NNSA (NN), DOE-EM (EW), and DOD. See Table IV.8.

Table IV.8 Nonproliferation Technologies
($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	3.4	4.3	4.3	4.5	4.5	4.5	4.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	3.4	4.3	4.3	4.5	4.5	4.5	4.5
Direct Personnel	6.0	9.0	9.0	9.0	9.0	9.0	9.0

Initiative: Nuclear Fuel Cycle Technology Applications

Argonne is a leader in the technology of the nuclear fuel cycle. This initiative proposes application of our expertise and facilities to reducing the likelihood of diversion of nuclear materials throughout the nuclear fuel cycle, to identifying materials detected in illicit commerce, and to characterizing materials that might be encountered in a nuclear incident.

Methodology for Nuclear Fuel Cycle Observability and Transparency. Observability and transparency are critical objectives in improving the proliferation resistance of existing and future nuclear fuel cycles. Advanced nuclear fuel cycles must be designed to maximize those attributes for the facilities of all IAEA member states that do not already possess nuclear weapons. Initially designing fuel cycle processes and operations to be more observable and transparent reduces the potential for undetected proliferation. A formal methodology for implementing greater observability and transparency facilitates integration of attributes inherent in plant operation with advanced technologies for information management and unattended monitoring. Such integration will enable timely verification that only declared operations are being conducted within declared facilities. This kind of advanced methodology combines positive verification (i.e., material accountancy) with negative verification (i.e., operations accountancy) to increase the effectiveness of safeguards.

Nuclear Material Attribution. The ability to determine (1) where nuclear materials originated, (2) the capabilities by which they were produced, and (3) the ways in which they might be used is important for interdicting illicit commerce in nuclear materials and for determining the source of nuclear materials obtained by terrorists. We propose to apply our expertise in nuclear fuel cycles to these three tasks as an expansion of our current work on materials attribution for homeland defense.

Nuclear Material Characterization. Emergency response and mitigation in response to a terrorist attack involving a radiological dispersion device or a crude nuclear device require knowledge of the character of the materials involved and the phenomenology of the device. We propose to apply our expertise to planning for the characterization of materials produced from such a device (e.g., by understanding the materials' signatures), identifying possible pathways to communities and the environment, and developing means of mitigating impacts.

Resources for this initiative will be sought from DOE-Defense Nuclear Nonproliferation (NN), DOD, and other agencies involved in homeland defense. See Table IV.9.

Table IV.9 Nuclear Fuel Cycle Technology Applications ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	2.0	2.5	2.5	2.5	2.5	2.5	2.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	2.0	2.5	2.5	2.5	2.5	2.5	2.5
Direct Personnel	9.0	11.5	11.5	11.5	11.5	11.5	11.5

Initiative: Training for Specialists in Nuclear Material Protection and Law Enforcement

For several years we have supported the MPC&A program of NNSA by providing training to nuclear security personnel from Russia and the independent FSU countries. This training, conducted at the MPC&A Training Facility at Argonne-West, teaches the latest security concepts and gives students hands-on experience in operating electronic and computerized security systems. In coming years, we will offer to expand the number of classes conducted and thereby enable NNSA to accelerate completion of its MPC&A projects. In addition, we will offer our security training facility and expertise to help law enforcement officials meet their homeland security responsibilities. We are currently discussing with local law enforcement officials their training needs related to access control for courts, public buildings, and airports.

In addition to offering security experts for foreign projects, we stand ready to provide experts for surveys supporting homeland security.

Resources required are summarized in Table IV.10. Funding will be sought from DOE-Defense Nuclear Nonproliferation (NN).

Table IV.10 Training for Specialists in Nuclear Material Protection and Law Enforcement
($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	2.5	3.0	3.5	3.5	3.5	3.5	3.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	2.5	3.0	3.5	3.5	3.5	3.5	3.5
Direct Personnel	5.0	6.0	6.5	6.5	6.5	6.5	6.5

Initiative: International Nuclear Safety and Cooperation

We support the International Nuclear Safety and Cooperation program, which assesses the safety of Soviet-designed power reactors. This work has demonstrated the need for continued U.S. engagement with less developed countries seeking peaceful use of nuclear technologies. Moreover, this ongoing program has revealed important nuclear safety and security issues that indicate threats to these reactors. Therefore, we propose to expand our current program to collaborate with countries wishing to assess and address such issues. The focus of the program will be assessments of the risks facing nuclear installations from both internal and external threats. The program would include collaborative training, coordinated between Argonne and the IAEA, that facilitates the transfer of safety assessment technology to participating countries, as well as the linking of those countries into the network of international nuclear safety centers.

Resource requirements are given in Table IV.11. NNSA funding (AF-15-30) would be supplemented by funding from the U.S. Agency for International Development and from the Nonproliferation and Disarmament Fund.

Table IV.11 International Nuclear Safety and Cooperation ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	0.4	1.0	1.0	1.0	1.0	1.0	1.0
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	0.4	1.0	1.0	1.0	1.0	1.0	1.0
Direct Personnel	1.5	3.0	3.0	3.0	3.0	3.0	3.0

Initiative: Integrated Research Reactor Safety Enhancement Program

We propose to significantly expand our work in the area of cooperation and safety enhancement for international research reactors. Research reactors represent unique safety and security risks for less developed countries. An integrated approach to addressing these risks — based on our experience in work with research reactors, international safety networks, fuels, and decommissioning — can offer NNSA a more powerful way to improve research reactor safety. By leveraging existing safety infrastructures, we can approach facilities of concern in a cooperative manner, assess vulnerabilities, and provide substantial assistance in the areas of fuel characterization, stabilization, and disposition;

safety and security upgrades; safety infrastructure development; and emergency preparedness.

We have a long history of working with the owners and operators of foreign reactors and their support organizations to assess and improve nuclear safety. Establishment of networked international nuclear safety centers will continue to provide valuable liaisons with the nuclear communities in the countries of the FSU and elsewhere. This network can provide the framework for reducing risks associated with research reactors and can offer valuable support in areas such as emergency response and health physics training. Many research reactor facilities worldwide suffer from poor quality assurance programs, lack of trained personnel, insufficient safety reviews, and limited regulatory oversight. Working in parallel with the new International Nuclear Safety and Cooperation program proposed above, the Integrated Research Reactor Safety Enhancement Program can address both broader infrastructure issues and specific facility issues.

Synergies with existing Argonne work for the RERTR program and for material protection programs will be exploited to provide maximum benefit to NNSA. Cooperation with the IAEA and the U.S. Nuclear Regulatory Commission will further enhance the program's effectiveness.

Resource requirements are given in Table IV.12. NNSA funding (NN-30) may be supplemented with funds from the U.S. Agency for International Development and from the Nonproliferation and Disarmament Fund.

Table IV.12 Integrated Research Reactor Safety Enhancement Program ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	1.9	3.0	3.5	3.5	3.5	3.5	3.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	1.9	3.0	3.5	3.5	3.5	3.5	3.5
Direct Personnel	2.5	5.0	7.0	7.0	7.0	7.0	7.0

b. Infrastructure Assurance and Counterterrorism

Situation

Our work on infrastructure assurance and counterterrorism aims to assure the security and reliability of critical U.S. infrastructures and other key national assets — as well as the safety of associated populations — that are threatened by disruptions resulting from natural events, accidents, or deliberate acts such as terrorist attacks. This work addresses cyber security and technologies, as well as capabilities for detecting, combating, and recovering from chemical, biological, and nuclear terrorism (a growing national security concern addressed in the preceding Nuclear National Security area plan, Section IV.A.3.a). Work in these areas of homeland security directly supports both DOE's overarching national security mission and the mission of the new Department of Homeland Security (DHS).

Our work on infrastructure assurance and counterterrorism draws on expertise, knowledge, technologies, and specialized research facilities developed over decades for other purposes. By leveraging our core science and technology competencies, this work responds to the shifting challenges facing the nation. These challenges are complicated by changes in threat profiles, weapons, targets, attackers, and motivations.

Our infrastructure assurance and counterterrorism programs have annual budgets totaling approximately $12 million. Significant components of these programs include the following:

- The Vulnerability Assessment program evaluates the safety and security of critical infrastructure by considering physical security, operations security, cyber security, and infrastructure interdependencies. The program includes comprehensive assessments and rapid surveys.
- The Energy Infrastructure Interdependencies program evaluates the

interdependencies among various types of infrastructures (e.g., between electric power and natural gas or between electric power and telecommunications); the potential for cascading impacts resulting from disruptions to one or more types of infrastructures; better methods of detecting events affected by infrastructure interdependency; and improved technologies and procedures for preventing, responding to, and recovering from such events.

- The Infrastructure Outreach program increases the awareness of infrastructure owners and operators concerning security issues. This program also promotes sharing of best practices and lessons learned in infrastructure assurance.

- The Community Critical Infrastructure Protection program, in collaboration with community emergency planners and local utilities, develops plans and procedures that municipalities can use to prevent, respond to, and recover from major disruptions to energy infrastructure (e.g., that for electric power or natural gas).

- The Interior Infrastructure Protection for Chemical/Biological Attacks program demonstrates technologies for mitigating impacts from chemical or biological attacks on interior infrastructure deemed to be at above-average risk, such as subways, airports, and public buildings.

In addition to the programs described above, we maintain the following significant capabilities and facilities for addressing potential chemical and biological threats:

- Instruments for detecting potential chemical or biological threats in air, water, and soil, whether dispersed over kilometers or hidden in caches.

- Facilities for evaluating the effectiveness of chemical and biological monitoring methods, at both laboratory scale and field scale.

- Capabilities for determining health and environmental risk from the dispersion of chemical, biological, and nuclear weapons.

- Capabilities for evaluating the effects of agents on materials and for developing protective materials and methods of decontamination.

- Laboratories and expertise for developing prophylactic drugs and vaccines based on structural analyses of biomolecules.

- Fast-response systems for protecting first responders, decreasing exposure times, and reducing risk.

- The capability to conduct laboratory and field analyses enabling attribution of chemical or biological attacks.

- The Electron Microscopy Center, which provides high-resolution scanning electron microscopes able to examine and characterize the nanoscale embodiments likely to be used in chemical and biological detectors.

- The Multi-Bay Robotics Laboratory, which can develop robotic manipulator systems for remote work in unstructured hazardous environments.

- The Mobile Laboratory for Chemical Agent Detection, which is used to characterize chemical agent contamination in U.S. Army buildings. Samples can be analyzed on-site for rapid turnaround, and the facility can confirm decontamination after cleanup operations.

- The Dilute Chemical Agent Facility, which is approved by the U.S. Army to Level 2 and is certified to accept agents such as soman, sarin, and lewisite. The facility is equipped for development of analytical methods, detector testing, development of decontamination technologies, and validation of transport models. This facility currently serves as an emergency response laboratory for the Environmental Protection Agency.

Other Argonne facilities also provide significant R&D capabilities for addressing potential chemical and biological threats. These include the APS and the associated Structural Biology Center and Midwest Center for Structural Genomics. Though most of the Laboratory capabilities and facilities identified here were not specifically established for R&D related to chemical and biological counterterrorism, they nevertheless are significant resources for addressing currently anticipated threats.

Mission

By leveraging our expertise and facilities, both physical and computational, we support DOE's overarching national security mission and the complementary efforts of other federal agencies to ensure the security and reliability of the nation's critical infrastructure and reduce threats from weapons of mass destruction.

Issues and Strategy

In the area of infrastructure assurance and counterterrorism, we support the development of technologies and strategies that improve detection, mitigation, response, and recovery. As described below, we plan to expand our work on infrastructure vulnerability and risk assessment, energy systems analysis, analysis of infrastructure interdependencies, emergency preparedness, consequence management, and protection from chemical and biological threats. These activities have been given high priority by DHS and the White House Office of Science and Technology Policy, and they are cornerstones of DOE's long-term R&D program on critical infrastructure protection.

In the area of counterterrorism, we continue to expand research related to chemical and biological threat analysis, vulnerability assessment, detection and speciation, and incident response and attribution. These activities are based on Argonne competencies that include (1) molecular biology, (2) structural analysis, (3) radiation chemistry and photochemistry, (4) catalysis and electrochemistry, and (5) chemical and biological decontamination. For example, a microchip-type sensor that employs methods for isolating and labeling RNA (ribonucleic acid) is being evaluated as part of a comparative study sponsored by the Defense Threat Reduction Agency. We are also developing other detection methodologies that rely on biomolecular recognition, antibody pairing, or molecular fluorescence. Further current research focuses on ozone-based decontamination systems, aerosol monitoring, and risks associated with chemical warfare agents. During the coming year, we will submit new threat reduction initiatives to DOE and other concerned public agencies. These initiatives are based both on our expertise and on facilities such as the APS, the Structural Biology Center, and the Midwest Center for Structural Genomics.

Important recent developments in Argonne's work on counterterrorism are two NIH-funded entities: the Midwestern Regional Center of Excellence for Biodefense and Emerging Infectious Diseases Research (RCE) and the Regional Biocontainment Laboratory (RBL). The RCE, being led by the University of Chicago and Northwestern University, involves multiple universities, research institutes, and public health authorities and more than 100 scientists. The RBL will provide RCE researchers with facilities certified to "biosafety level 3" (the third highest of four levels). See Section S1.C for further information.

Initiative: Infrastructure Assurance and Counterterrorism

We propose to expand our current research, development, and analysis activities in the area of critical infrastructure assurance and counterterrorism. The goal of this work for DOE, DHS, and other federal agencies is to develop and apply innovative technologies, methodologies, models, and simulations that (1) will better protect critical U.S. infrastructure (including cyber-based information systems) and associated populations from disruption and (2) where disruptions do occur, will improve detection, mitigation of effects, response, and recovery. Our capabilities are particularly relevant to the infrastructures for energy (electric power, oil, and natural gas), transportation, agriculture, water supply, information and communications, and emergency services.

This initiative responds to major documents outlining U.S. policy toward homeland security, including the *President's National Strategy for Homeland Security* (July 16, 2002), the *USA Patriot Act of 2001*, and the *National Strategy for the Physical Protection of Critical Infrastructures and Key Assets*. The initiative is also consistent with the strategic thrust of DOE's Office of Energy Assurance, which was established in December 2001 to serve as the focus for DOE's activities in energy infrastructure assurance. Under these executive orders, DOE is the lead federal agency for assuring the continuity and viability of the nation's critical energy infrastructures.

Our long history of work related to infrastructure assurance and counterterrorism — reinforced by more intensive work over the past five years for the DOE Office of Energy Assurance, the Critical Infrastructure Assurance Office, DOD, and other government organizations — provides the foundation for this initiative. We will expand our work in the areas of vulnerability and risk assessment, energy and water systems analysis, information management, infrastructure interdependencies analysis, modeling and simulation of agent-based and complex adaptive systems, decontamination and remediation, and emergency preparedness and consequence management.

Improved technologies and capabilities are needed in all these areas to address the unprecedented range of physical and cyber threats to critical U.S. infrastructure from natural causes, accidents, and deliberate acts like the terrorist attacks on the World Trade Center and Pentagon. We will particularly emphasize development of methodologies and tools for analyzing the new vulnerabilities that have arisen because various components of the nation's infrastructure have become increasingly complex, automated, physically interconnected, and logically interdependent. The White House Office of Science and Technology Policy has given high priority to research on interdependent infrastructure, a cornerstone of DOE's long-term program on critical infrastructure protection.

We will continue to enhance our collaboration with other national laboratories as we conduct vulnerability surveys and assessments and develop cost-effective solutions to infrastructure assurance and counterterrorism problems. In the area of chemical and biological threats, we are currently leading multilaboratory teams of experts in modeling and analyzing infrastructure interdependencies and protecting civilian interior infrastructures (such as subway systems, airports, and public buildings) deemed to be at above-average risk.

Resources required for this initiative are summarized in Table IV.13. Funding will be sought from the DOE Office of Energy Assurance (GD-05), the NNSA Office of Defense Nuclear Nonproliferation (NN-20), other DOE program offices, and other federal agencies.

Table IV.13 Infrastructure Assurance and Counterterrorism ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	13.0	12.0	12.0	12.0	12.0	12.0	12.0
Capital Equipment	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Construction	-	-	-	-	-	-	-
Total	13.1	12.1	12.1	12.1	12.1	12.1	12.1
Direct Personnel	60.0	55.0	55.0	55.0	55.0	55.0	55.0

c. Department of Homeland Security

Situation

Recent terrorist attacks on the United States and heightened threats resulting from the liberation of Iraq have underscored the need for increased emphasis on homeland security. The most recent immediate concern is the possibility that terrorist groups have obtained nuclear, biological, or chemical weapons — or their constituents — from Iraq. Addressing challenges from the unconventional weapons and delivery methods used by terrorist organizations will be a high national priority for the foreseeable future. To anticipate, detect, defend against, mitigate, and recover from such attacks — whether directed against domestic civilian populations, economic targets, or critical elements of the nation's infrastructure — the United States must both adapt existing security systems and implement new planning methods, new detection and monitoring systems, new communication and control processes, new remedial technologies, and new analytical methods.

With the other national laboratories, Argonne already supports post-911 national security research through programs funded by DOE and other government agencies. As indicated in the two area strategic plans above, our current diverse research on science and technology for nuclear nonproliferation, arms control, infrastructure assurance, and counterterrorism is based on expertise, experience, and facilities that were developed over decades to support the DOE mission. Other relevant R&D efforts and assessments for non-DOE agencies include work for DOD, the Environmental Protection Agency, and the Federal Emergency Management Agency in the areas of planning and technology for environmental health, infrastructure assurance, and counterterrorism.

Though many of these ongoing R&D activities are directly relevant to the mission of the new DHS, in April 2003 few Argonne programs were directly sponsored by DHS. We anticipate that more existing programs will be transferred to DHS by their current sponsors and that new DHS programs will be established.

Mission

We will apply Argonne's technical and analytical expertise, resources, and facilities — in physical, biological, and computational science and technology — to help DHS pursue its mission to reduce threats to U.S. populations, communities, and infrastructure resulting from terrorism, especially terrorism involving weapons of mass destruction and weapons capable of causing massive disruption.

Issues and Strategies

We have technical capabilities in a number of research areas that are highly relevant to the DHS mission, notably in the areas of nuclear, biological, and chemical instruments and sensors; analytical chemistry and biology; attribution analysis; applied computational methods; health and environmental risk assessment; detection, handling, and containment of hazardous nuclear, chemical, and biological materials; decontamination of sites and facilities; advanced materials technology; infrastructure protection planning; structural biology and genomics; biological detectors; robotics; and logistics systems analysis. We are also equipped to provide technical support for certain rapid response functions related to the DHS mission.

As its responsibilities and priorities are better defined, we plan to propose to DHS new R&D initiatives that are consistent with the Laboratory's mission, its responsibilities to DOE, and its core competencies. In preparation, Argonne has appointed an acting associate laboratory director with specific responsibility for organizing, focusing, and structuring the Laboratory's programs in homeland security and other areas of national security. Future editions of Argonne's *Institutional Plan* will spell out in more detail our current and planned work for DHS.

4. Collaborative R&D Partnerships

Situation

If our research is to have an impact and provide benefits, results must be readily accessible to commercial firms for further development and application to meet the needs of industry and the public. We pursue these objectives through broad publication of results, development of patent portfolios, and partnering with industry. Our research partnerships with industry contribute strongly to DOE's strategic goals and provide a basis for U.S. innovation.

As part of our focus on partnerships, we have expanded our collaboration with the University of Chicago through numerous joint research projects. The technology transfer offices at the two institutions work together to identify the most effective approaches to commercializing Argonne intellectual property. Day to day, Argonne's Technology Transfer Office works closely with Laboratory research divisions to develop productive research contracts with partners in industry, academia, and not-for-profit organizations, in order to provide competitive benefits to users of Argonne technologies and, ultimately, enhanced energy security and environmental quality for the nation.

Mission and Vision

The mission and vision of our technology transfer program include five elements:

- Enhance the competitiveness of U.S. industry by transferring Argonne technology solutions to industry and the marketplace.

- Expand and enhance Argonne's R&D programs and funding through cooperative research and technical interactions with government, academic, and private organizations.
- License Argonne intellectual property to enhance U.S. competitiveness while providing revenue to the Laboratory.
- Foster utilization of Argonne's R&D through proactive efforts to deploy results to industry and, ultimately, provide benefits to the public.
- Leverage technology transfer to increase returns to Argonne and significantly contribute to the Laboratory's fulfillment of its mission and strategic goals; to this end, use joint ventures, new company start-ups, and other productive business arrangements.

Approach

We use a variety of tactical approaches to accomplish our mission and provide benefits to the nation. Most importantly, we support numerous cooperative R&D agreements (CRADAs) through Laboratory research programs. Increasingly, we use work-for-others contracts as a vehicle for industrial agreements and transfer of our technology. In addition, we use "full funds-in CRADAs" as a basis for developing cooperative research partnerships that move Laboratory technologies toward commercialization. In FY 2002 Argonne initiated a joint program with the University of Chicago to identify technologies particularly well suited to commercialization by start-up companies and then to take steps toward organizing appropriate new ventures that can attract funding from outside investors.

For further information about technology transfer at Argonne, see Supplement 2.

B. Laboratory Directed R&D Program

The Laboratory Directed Research and Development (LDRD) program funds creative and innovative R&D projects at Argonne. Selection of projects is the responsibility of the laboratory director. The objectives of LDRD are to stimulate innovation and creativity, to continuously renew the scientific and technological vitality of the Laboratory, and to respond to rapidly emerging R&D opportunities. The program enhances our ability to attract and retain the high-caliber scientists and engineers essential for undertaking our missions for DOE and the nation. In addition, LDRD helps ensure that we provide scientific and technical leadership in fields related to our mission.

Our primary criteria for selecting LDRD projects are scientific and technical excellence, innovativeness and cross-disciplinary character, relationship to Laboratory strategic goals and objectives, expected contributions from the results, and prospects for continuation under programmatic support. Each year the laboratory director designates portions of the LDRD budget for support of particular types of projects. Categories include (1) competitive grants initiated by a principal investigator or a team on any mission-related topic and (2) competitive projects directly relating to or supportive of the Laboratory's strategic initiatives. The immediate objectives of Argonne's LDRD portfolio are (1) to reinforce our R&D planning by supporting our mission and strategic view (as described in Chapter II of this *Institutional Plan*), (2) to enrich our technical capabilities, (3) to encourage innovation and creativity by technical staff through the development of new concepts and principles and the undertaking of projects having high risk but potentially high reward, and (4) to exploit Argonne's technical potential for the benefit of the nation. As a result of the criteria used to select projects, our portfolio of LDRD projects is clearly tied to DOE's overarching national security mission (encompassing science, energy, environment, and security). In addition, the LDRD program has the very important benefit of enhancing the morale and vitality of our scientific and technical staff. Researchers' enthusiasm is nurtured by the knowledge that good new ideas, even those well beyond existing programs, are eligible to compete for the immediate funding they need.

Our LDRD program supports promising novel and innovative projects wherever they may appear across the broad spectrum of science and technology relevant to current or prospective

Laboratory missions. A report of accomplishments across the entire LDRD program is made to DOE each year. Our notable recent accomplishments include the following:

- Developed a finite-difference time-domain approach to calculating the light-scattering cross sections of metal nanoparticles.
- Demonstrated the feasibility of applying to counterterrorism (1) the concepts of agent-based complex adaptive systems and (2) computer simulations.
- Fabricated, through both patterning and self-assembly, a variety of nanophotonic structures having novel optical properties.
- Demonstrated at bench scale a single-step lithium reduction process for uranium oxide that is applicable to the reduction of spent oxide reactor fuel to metal.
- Reduced to 120 nanometers the lower wavelength limit of x-rays produced in the free-electron laser at the APS, thereby creating an unrivaled x-ray source for photo-ionization experiments and for studying self-amplified spontaneous emission phenomena.
- Successfully applied advanced search algorithms and artificial intelligence codes to elucidate protein structure as determined by amino acid sequences and “fold-templates.”
- Developed a new process for removing hazardous organic compounds from ground-water by using a method exploiting centrifugal contactor-based solvent extraction.
- Developed a “phantom head” experimental model for studying cooling of the human brain as an emergency medical protocol.
- Developed the Open Link concept for efficiently linking computer codes and modules for environmental assessment.

The larger component of our LDRD emphasizes R&D aligned with Laboratory strategic initiatives, as reflected in this *Institutional Plan*. Strategic goals are periodically revised and reevaluated, as required. The specialized expertise of our staff naturally causes a substantial number of LDRD projects suggested by employees to fall into the various high-priority initiative areas, so they become eligible for a correspondingly high priority in the proposal selection process. As discussed in Chapter III, current major Laboratory initiative areas include Nanosciences and Nanotechnology, the Rare Isotope Accelerator, Functional Genomics, Petaflops Computing and Computational Science, Advanced Nuclear Fuel Cycle, and Hydrogen Research and Development.

Several LDRD projects will be supported under the auspices of the Competitive Grants component of the LDRD program. This component provides a direct avenue for single investigators and small multidisciplinary teams to propose projects to the laboratory director that do not fall within the Laboratory’s defined strategic initiative areas, but that have high scientific or technical merit and are at the forefront of their fields. A Director’s Review Committee, comprising scientists and engineers spanning the breadth of our disciplines and programs, subjects Competitive Grants proposals to a thorough and highly competitive merit review. The resulting ranking is used by the laboratory director to select winning proposals.

The LDRD program is funded Laboratory-wide through Argonne’s indirect budget. As part of our LDRD planning before each fiscal year begins, we propose to DOE a maximum total LDRD expenditure. As indicated in Table IV.14, for FY 2003-FY 2004 this upper limit generally approximates 4.5% to 5.0% of our projected total of operating and equipment funding.

Table IV.14 Laboratory Directed R&D Funding ($ in millions)

	FY01[a]	FY02[b]	FY03[c]	FY04[c]
	20.9	20.9	22.5	25.0

[a] Actual expenditures.

[b] Authorized maximum expenditures for the LDRD program.

[c] Proposed maximum expenditures for the LDRD program.