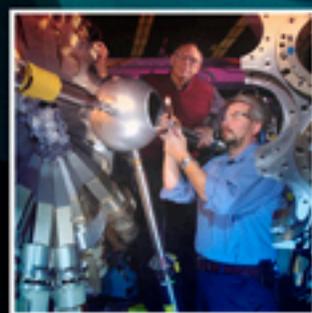
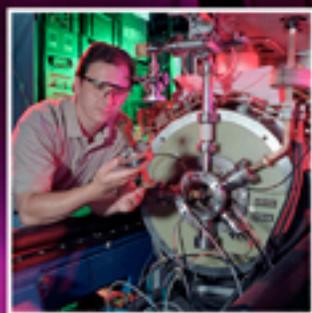


OCTOBER 2004

ANL/IP-2004

# ARGONNE NATIONAL LABORATORY INSTITUTIONAL PLAN



*Accomplishing DOE Missions*



## *On the Cover:*

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Argonne National Laboratory researchers celebrate the International Year of Physics with world-class nuclear physics research at ATLAS (the Argonne Tandem-Linac Accelerator System) and elsewhere (from left):

- An Argonne technician adjusts the ATLAS Electron Cyclotron Resonance source, which provides ions that are accelerated into the research beam. ATLAS, the world's first superconducting ion accelerator and a model for accelerators throughout the world, is capable of accelerating all of the natural elements.
- In research elsewhere, scientists from Argonne and McGill University adjust electronics circuitry on a Penning trap, used to measure the masses of nuclei.
- The ATLAS resonator constitutes the accelerator's heart.
- The Gammisphere, a detector used with ATLAS, is in the *Guinness Book of World Records* as the world's most powerful spectrometer for nuclear structure research.

Argonne National Laboratory

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# INSTITUTIONAL PLAN

ANL/IP-2004

Operated by The University of Chicago for the  
U.S. Department of Energy under Contract W-31-109-Eng-38

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October 2004

This October 2004 *Institutional Plan* was originally prepared in the early spring of 2004. It generally describes the activities and plans of Argonne National Laboratory as of that time. Thus, for example, financial data for FY 2004 are midyear projections.

Available electronically at this location: <http://www.ipd.anl.gov/instplan/>

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Argonne National Laboratory is operated by The University of Chicago for the United States Department of Energy's Office of Science.

# Contents

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<b>I. Laboratory Director’s Statement .....</b>	<b>I-1</b>
<b>II. Mission, Roles, and Strategic Goals .....</b>	<b>II-1</b>
<b>A. Mission .....</b>	<b>II-1</b>
<b>B. Vision.....</b>	<b>II-1</b>
<b>C. Scientific and Technical Core Competencies .....</b>	<b>II-4</b>
<b>D. Roles in Accomplishing DOE Missions.....</b>	<b>II-4</b>
<b>E. Strategic Context and Planning Assumptions.....</b>	<b>II-7</b>
<b>F. Strategic Objectives .....</b>	<b>II-8</b>
<b>III. Major Laboratory Initiatives.....</b>	<b>III-1</b>
<b>A. Science .....</b>	<b>III-1</b>
1. Nanosciences and Nanotechnology — Center for Nanoscale Materials .....	III-1
2. Rare Isotope Accelerator .....	III-3
3. Functional Genomics .....	III-5
4. Petaflops Computing and Computational Science .....	III-7
<b>B. Energy .....</b>	<b>III-9</b>
1. Advanced Nuclear Energy Systems .....	III-9
2. Hydrogen Research and Development.....	III-11
<b>IV. Science and Technology Strategic Plan.....</b>	<b>IV-1</b>
<b>A. Fundamental Science and National Research Facilities.....</b>	<b>IV-1</b>
1. Advanced Photon Source.....	IV-1
2. Materials Science.....	IV-7
3. Chemical Sciences .....	IV-10
4. Nuclear Physics and the Argonne Tandem-Linac Accelerator System.....	IV-13
5. High-Energy Physics .....	IV-14
6. Mathematics, Computing, and Information Sciences.....	IV-16
7. Intense Pulsed Neutron Source .....	IV-18
8. Biosciences .....	IV-20
9. Environmental Research .....	IV-22
10. Science and Engineering Education and University Programs .....	IV-25
<b>B. Energy and Environmental Technologies .....</b>	<b>IV-27</b>
1. Advanced Nuclear Technology.....	IV-27
2. Energy and Industrial Technologies .....	IV-29
3. Transportation Technologies .....	IV-33
4. Environmental Treatment Technologies .....	IV-35

---

5. Energy and Environmental Systems.....	IV-39
6. Biotechnology.....	IV-42
<b>C. National Security.....</b>	<b>IV-43</b>
1. Nuclear National Security.....	IV-43
2. Homeland Security .....	IV-48
3. National Defense .....	IV-51
<b>D. Collaborative R&amp;D Partnerships .....</b>	<b>IV-52</b>
<b>E. Laboratory Directed R&amp;D Program.....</b>	<b>IV-53</b>
<b>V. Operations and Infrastructure Strategic Plan .....</b>	<b>V-1</b>
<b>A. Human Capital .....</b>	<b>V-2</b>
<b>B. Site and Facilities .....</b>	<b>V-4</b>
<b>C. Environment, Safety, and Health.....</b>	<b>V-7</b>
<b>D. Integrated Safeguards and Security Management.....</b>	<b>V-9</b>
<b>E. Information Management.....</b>	<b>V-11</b>
<b>F. Communications, Outreach, and Community Relations .....</b>	<b>V-14</b>
<b>G. Performance Management .....</b>	<b>V-16</b>
<b>VI. Resource Projections.....</b>	<b>VI-1</b>
<b>Supplement 1: Work for Sponsors other than DOE.....</b>	<b>S1-1</b>
<b>A. Nuclear Regulatory Commission .....</b>	<b>S1-1</b>
<b>B. Department of Defense .....</b>	<b>S1-3</b>
<b>C. Department of Health and Human Services .....</b>	<b>S1-7</b>
<b>D. Other Federal Agencies .....</b>	<b>S1-9</b>
<b>E. Nonfederal Organizations .....</b>	<b>S1-13</b>
<b>F. Department of Homeland Security .....</b>	<b>S1-16</b>
<b>Supplement 2: Technology Transfer .....</b>	<b>S2-1</b>
<b>A. R&amp;D Agreements .....</b>	<b>S2-1</b>
<b>B. Licensing .....</b>	<b>S2-1</b>
<b>Supplement 3: Other Tables.....</b>	<b>S3-1</b>
<b>A. Science and Math Education.....</b>	<b>S3-1</b>
<b>B. User Facilities .....</b>	<b>S3-1</b>

**Organization Chart**

# I. Laboratory Director's Statement

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As a member of the national laboratory system for more than 58 years, Argonne conducts world-class research and development in support of the long-term goals of the Department of Energy (DOE) and its Office of Science, to “position our nation for scientific and economic strength and leadership in the years to come.” Our efforts focus on basic science, energy resources, environmental stewardship, and national security.

To enhance our performance in carrying out DOE's missions, Argonne and the University of Chicago — which has operated the Laboratory for its entire history — work closely together to strengthen ties and increase research collaboration between the two institutions.

Argonne manages five major DOE user facilities, and we are working to add to this roster. We work with colleagues from the other national laboratories, academia, and industry to employ these national research tools on the cutting edge of science and technology.

The key to making our discoveries useful is to move them quickly from the laboratory to the marketplace. Our current portfolio of technologies contains approximately 185 patents and copyrighted software products available for licensing by private enterprise. It also includes substantial efforts for the Department of Homeland Security (DHS). Our support for DHS draws on our deep understanding of the nation's technology infrastructure and on application of our technologies to detect, prevent, and retaliate against terrorist attacks.

## National User Facilities

Over the decades, Argonne and other members of the national laboratory system have proven highly effective at planning, designing, building, and operating user facilities. These one-of-a-kind research centers serve as engines that help maintain and advance U.S. scientific leadership by attracting the world's best scientists and providing crucial support for national communities of researchers in many fields. The

following major national user facilities are currently operated by Argonne for DOE, or are in the planning stages:

- The *Advanced Photon Source* (APS) is our premier user facility. It provides researchers with the nation's brightest x-ray beams for investigations in a broad spectrum of scientific and technological areas, including materials science, structural biology, environmental studies, and applied engineering. Collaborative access teams — comprising investigators from private industry, universities, government, and other institutions — have committed a quarter of a billion dollars in capital investments for construction of APS beamlines.
- The *Intense Pulsed Neutron Source* (IPNS) is widely known as one of DOE's exemplary user facilities, particularly because the machine and its operators embody the professional values of its national user community and assiduously serve the community's scientific interests. In the 23 years since its inaugural run, the IPNS has become a national model for user facility operations. In recent years, the organization and its staff have committed their expertise to supporting the Spallation Neutron Source (SNS) project — soon to become the nation's premier neutron source — by designing and building instruments for the SNS and by training future SNS users.
- The *Argonne Tandem-Linac Accelerator System* (ATLAS) is the world's first superconducting linear accelerator for heavy ions and the premier accelerator for low-energy nuclear physics research. In addition to supporting an active and productive community of physicists from all over the world, ATLAS plays a key role in our conceptual design for the proposed Rare Isotope Accelerator (RIA).
- The *Electron Microscopy Center* (EMC) conducts materials research using advanced microstructural characterization methods and

state-of-the-art microscopes. Research by EMC personnel includes microscopy-based studies of high-temperature superconducting materials, irradiation effects in metals and semiconductors, phase transformations, and the structure and chemistry of thin-film interfaces.

- The *Atmospheric Radiation Measurement (ARM) Climate Research Facility* is DOE's largest research program on global climate change. ARM Program scientists focus on obtaining field measurements and developing models to better understand the processes that control solar and thermal infrared radiative transfer in the atmosphere, especially in clouds and at Earth's surface.
- The *Center for Nanoscale Materials (CNM)*, one of five Nanoscale Science Research Centers sponsored by DOE, concentrates on understanding and controlling material properties at the nanometer scale. This area of scientific exploration has tremendous potential to advance science and technology. The CNM already offers advanced facilities and expertise to support independent and collaborative research efforts, and construction of a dedicated building adjacent to the APS has begun. The CNM focuses on six primary research themes: bio-inorganic interfaces, complex oxides, nanocarbon, nanomagnetism, nanophotonics, and theory and simulation.

In addition, Argonne will be the site of the Ricketts Center, a Regional Biocontainment Laboratory funded by the National Institutes of Health to study the detection, prevention, and treatment of infectious diseases — particularly agents that could be used for bioterrorism. The Ricketts Center, in conjunction with the APS and CNM, will form one of the world's most complete complexes for microbiological research.

### **Core Competencies and Major Initiatives**

Our major strategic goals are supported by our core competencies, which we constantly strengthen. Chief among our competencies are our world-class engineering and scientific expertise in producing safe, sustainable, proliferation-resistant nuclear energy and our long experience and deep

expertise in developing, operating, and advancing the science and technology underpinning accelerator-based user facilities. We also have widely recognized expertise in the materials sciences; chemistry; biology; physics; high-energy and nuclear physics; cross-disciplinary nanoscience and technology; structural biology, functional genomics, and bioinformatics; applied mathematics and computer science; computational science; and environmental science. Our overall goal is to be the best in the world in many areas, a leader in others, and a responsible steward of our facilities.

To complement existing programs, we work closely with DOE and the scientific community — often in a leadership role — to develop new initiatives and scientific facilities to serve national needs. The following six Argonne initiatives represent timely opportunities to significantly enhance U.S. research capabilities in basic research and development and, hence, to advance scientific understanding and engineering achievement across a wide range of disciplines:

- *Nanosciences and Nanotechnology.* Research on nanoscale materials will lead to devices such as computers that are smaller and more efficient and to materials with exciting new properties. Argonne is well positioned to contribute to achieving these national goals and is actively developing regional collaborations to help.
- *Rare Isotope Accelerator.* By accelerating highly unstable nuclei at the very limits of existence, RIA will open new scientific frontiers. Examination of these isotopes and their reactions will answer important astrophysical questions, such as how stars evolve, how their evolution affects the evolution of galaxies and planets, and how much “ordinary” matter the universe contains. Physicists will study the fundamental nuclear processes by which stars generate energy and create heavy elements; discover new and unexpected phenomena; and develop new approaches to studying nuclear decay, reactions, and structure. In collaboration with Michigan State University and other institutions, we have developed a facility concept for RIA that achieves its physics goals at reasonable cost by incorporating our

existing state-of-the-art heavy-ion accelerator, ATLAS.

- *Functional Genomics.* Recent developments in genome-wide DNA sequencing, high-throughput analytical tools, and computing technologies have made feasible the genome-wide analysis of biomolecular function. Such research promises new strategies for altering cellular activities in order to improve human health, environmental management, and economic productivity. It also will help DOE pursue its homeland security mission by deepening understanding of organisms used as biological warfare agents. To address this opportunity, we are developing a major Laboratory initiative to undertake large-scale functional analyses of macromolecules and macromolecular complexes. We are also strengthening our research staff to contribute to this fast-moving field. A partnership between our Biosciences Division and our Mathematics and Computer Science Division will coordinate the efforts of experimentalists and simulation experts to develop exciting new capabilities in bioinformatics and computational cell biology.

- *Petaflops Computing and Computational Science.* We are building on our existing long-term program in mathematics and computer science to support work in the areas of mathematical software, parallel programming tools, advanced visualization systems, grid computing and distributed systems, collaboration technologies, scalable systems software, and performance analysis and modeling. Strong internal and external scientific collaborations tie this computer science research to diverse applications in biology, high-energy physics, climate modeling, computational chemistry, chemical engineering, subsurface modeling, biomedical computing, astrophysics, and other areas. Our initiative aims to accelerate progress in these areas through a Laboratory-wide computational science program, a targeted research and development program, and construction of a large-scale research facility to house a petaflops computing system and supporting programs in collaborative computational science research.

- *Nuclear Energy.* The nation's need for a secure, reliable supply of energy dictates that nuclear energy play a major role in the future. Our researchers are identifying technologies for the economical production of increasing amounts of energy while reducing burdens on the environment. This work includes addressing the problems of spent fuel disposition and nuclear nonproliferation inherent in producing nuclear energy on the required scale. In particular, we are looking at ways to return fuel to the reactor and produce more benign waste forms.

- *Hydrogen Research and Development.* In response to President Bush's national initiative to reverse growing dependence on foreign oil by developing the technology that could make hydrogen a viable and widely used fuel, we have mounted a coordinated effort integrating our state-of-the-art user facilities with our expertise in basic science and technology and in nearer-term technology development and deployment. Central to this program are two objectives that drive progress toward the hydrogen economy: (1) high-performance materials for hydrogen separation and fuel cell membranes and (2) new catalysts that improve hydrogen production and combustion. We are drawing on our broad knowledge of materials science and chemistry to orchestrate comprehensive research programs that coordinate advances across the spectrum from basic science to applications. In these efforts, the unique capabilities of the IPNS, APS, and EMC will be particularly valuable, and we will rely on our extensive expertise in nuclear reactor technology to investigate the production of hydrogen from nuclear power.

The state of Illinois has provided extremely valuable support for Argonne's major research initiatives. This outstanding cooperation has fostered a highly favorable environment for accomplishing the Laboratory's missions.

### **Employer of Choice**

The most important measure of an organization is the quality and dedication of its people. Our successes come from our staff. Many have been with Argonne for decades; more than a

quarter have 20 or more years of service. Obviously, Argonne is a good place to work. To strengthen our status as an employer of choice, we are pursuing a number of initiatives in our operations. One initiative is a human resources strategy to develop strong leadership, support a creative and diverse workforce, and recruit and develop the talent we need, in an environment totally committed to equal opportunity for everyone. Our development of talent begins at the earliest possible stage, with educational programs and other efforts to convey to students from grade school to the postdoctoral level our love of science and technology and our fascination with the possibilities they offer.

Notable among our operations initiatives are the following:

- Make optimal use of the national talent pool to attract the best qualified new employees from all ethnic and cultural backgrounds.
- Ensure that line managers are responsible for achieving excellent performance over the full range of activities under their purview. Our integrated management approach requires ongoing education and training of all staff.
- Maintain a safe and healthy workplace for our employees, with close attention to protecting the environment for the benefit of both ourselves and our neighbors. A bedrock principle is the empowerment of every

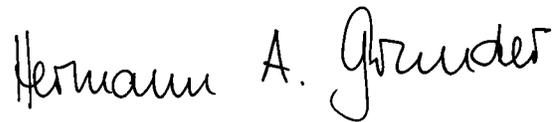
employee to object to any impediment to safety or security.

- Make open communications a key part of the Argonne culture, across all levels of management and staff. When communication flows unimpeded in all directions throughout an organization, resulting interactions produce fertile synergies and valuable new ideas. Line management needs this open communication to learn of all available good ideas and to help implement them.

### **Focus on the Ambitious**

Just as DOE's Office of Science has outlined an ambitious agenda for science, so has Argonne. We, too, dream large.

The goals of the Office of Science strategic plan fire our imaginations, and we embrace this exciting quest to advance the cutting edge of science, just as we have since our earliest days.



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Hermann A. Grunder  
Laboratory Director

## II. Mission, Roles, and Strategic Goals

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Argonne National Laboratory is a major multiprogram laboratory managed and operated for the U.S. Department of Energy (DOE) by the University of Chicago under a performance-based contract.

### A. Mission

Argonne's mission is to serve DOE and national security by advancing the frontiers of knowledge, by creating and operating forefront scientific user facilities, and by providing innovative and effective approaches and solutions to energy, environmental, and security challenges to national and global well-being, in the near and long term, as a contributing member of the DOE laboratory system.

We contribute significantly to DOE's mission in science, energy resources, environmental stewardship, and national security, with lead roles in the areas of science, operation of scientific facilities, and energy. In accomplishing our mission, we partner with DOE, other federal laboratories and agencies, the academic community, and the private sector.

### B. Vision

Argonne ensures U.S. scientific and technological leadership by creating — in the national interest — new knowledge and technologies that enhance energy security, national security, economic productivity, and quality of life. The Laboratory is a full participant in the implementation of administration priorities set forth by the President's science advisor. In all its programs, Argonne is committed to managing its resources to maximize benefit to the taxpayer, with DOE's critical performance measures as its guide.

Argonne's leadership inspires cooperation to integrate the resources of other laboratories, agencies, and universities to solve the nation's most challenging problems. The Laboratory's

scientific research supports every major DOE program. Our management approach is to focus the Laboratory's attention on research that has the greatest promise and highest potential impact for the coming decade. To maximize benefit to the nation, we create alliances with industry that expedite application of new discoveries and technological innovations.

Argonne is pursuing ten visionary *strategic goals* to deliver extraordinary science and technology with significant value to the nation:

1. Develop the technologies and infrastructure needed to produce, store, distribute, and use hydrogen fuel.
2. Close the nuclear fuel cycle, thereby reducing the need for multiple geologic repositories for nuclear waste and reducing the stockpile of weapons-grade plutonium and actinides.
3. Develop advanced nuclear power technologies that are safe, economical, proliferation-resistant, and environmentally sustainable.
4. Plan, design, construct, and operate the Rare Isotope Accelerator (RIA) and make fundamental discoveries in nuclear physics and astrophysics.
5. Construct and operate the Center for Nanoscale Materials and create innovative materials with valuable commercial properties.
6. Lead multilaboratory development of an end-to-end pilot to demonstrate the power of the Genomes to Life approach, develop world-class protein production and proteomics capabilities, and develop translational biology that spans the gap between molecular biology and its applications.
7. Realize the full potential of scientific simulation to solve mission-related problems, through leading-edge research on systems architecture and software, parallel programming and numerical tools, distributed

computing, and computational science applications.

8. Establish a new associate laboratory directorate in national security to deliver technologies and analyses for the Department of Homeland Security (DHS), the Department of Defense, the National Nuclear Security Administration, and the U.S. intelligence community.

9. Make major contributions to environmental research, taking full advantage of our state-of-the-art facilities and tools.

10. Optimize the operation of our national user facilities to perform research in fundamental science and other areas.

These strategic goals, explained more fully below, are consistent with priorities established in DOE's FY 2004 budget request.

### **Goal 1: Hydrogen Research and Development**

Argonne will help advance the basic science and technology development needed to produce, store, and distribute hydrogen and to use it in fuel cells, vehicles, and electricity generation. The Laboratory will focus its diverse intellectual resources, experimental capabilities, and user facilities to achieve breakthroughs in fundamental understanding of the materials and processes needed for a viable hydrogen economy. We will continue to participate in the FreedomCar partnership, in order to accelerate the development of practical, affordable hydrogen cell vehicles. We will perform the engineering and reactor physics required to develop a nuclear plant that co-generates hydrogen and electricity.

### **Goal 2: Advanced Nuclear Fuel Cycle**

Argonne will develop advanced technologies to treat spent nuclear fuel and transmute isotopes that contribute to long-term issues. We will design and demonstrate a fast-burner reactor to close the nuclear fuel cycle. This approach will reduce the need for geologic repositories, contribute to U.S. energy independence by recycling spent commercial nuclear fuel, and reduce the stockpile of weapons-grade plutonium and actinides.

### **Goal 3: Nuclear Energy**

Argonne will help develop advanced nuclear power technologies that are safe, economical, proliferation-resistant, and environmentally sustainable. We will help design and test the Next-Generation Nuclear Plant being contemplated by DOE. We will continue to support the fusion energy sciences with research in plasma and reactor physics and engineering.

### **Goal 4: Nuclear Physics and the Rare Isotope Accelerator**

Argonne will build and operate RIA as a forefront user facility, thereby opening new frontiers for research in nuclear physics and astrophysics and extending the Laboratory's tradition of innovation, scientific leadership, and service to facility users. RIA will allow us to obtain critical scientific information about how heavy elements are created and how nuclear properties influence the stars; the properties of short-lived atomic nuclei near their limits of stability; and the nature of nuclear decay, reactions, and structure.

### **Goal 5: Nanoscience and Nanotechnology**

Argonne will enable the rapid characterization of new materials required for the nanoscale revolution by co-locating multiple research disciplines and nanoscience instrumentation at two of its national user facilities: the Advanced Photon Source (APS) and the Intense Pulsed Neutron Source (IPNS). DOE has approved the mission need ("critical decision 0") and the preliminary baseline range ("critical decision 1") for Argonne's Center for Nanoscale Materials. Construction of this state-of-the-art user facility adjacent to the APS has begun. The state of Illinois is funding the building, and DOE is funding the scientific equipment, including a world-class nanoprobe beamline at the APS.

### **Goal 6: Bioscience**

To enable forefront research in structural and cell biology, functional genomics, and other areas, Argonne will develop world-class facilities for the production, crystallization, and characterization of

proteins. In general, we are planning for significant growth in research for DOE's Genomes to Life (GTL) program. We plan to lead a coordinated multilaboratory GTL research program that, in addition to generating important science, will demonstrate the power of the scientific approach exemplified by GTL facilities. By integrating protein production capabilities with capabilities in structural genomics, proteomics, computational biology, and molecular biology, the program will contribute to fundamental understanding of living systems. We will develop translational biology to span the gap between molecular biology and its applications. Expanding research at the interface of molecular biology and nanoscience will focus both on applying nanotechnology to study biomolecular systems and on using biomolecules to construct novel nanostructures. In a coordinated effort, Argonne has been chosen as the site for a Regional Biocontainment Laboratory — the Ricketts Center — that will conduct microbiology research to combat emerging infectious diseases and reduce threats from bioterrorism. This facility will be operated by a consortium led by the University of Chicago and funded by the National Institutes of Health.

#### **Goal 7: Advanced Scientific Computing**

Argonne will provide the high-performance computational and networking tools that are indispensable for scientific discovery. The Laboratory has had international impact through its leadership in the areas of Grid computing, scalable numerical tools, parallel computing, and advanced visualization. Moreover, we are strengthening our work on computational science applications, especially in the areas of nanoscience and biology. We will continue to support the Scientific Discovery through Advanced Computing program — a multidisciplinary effort involving teams of mathematicians, computer scientists, and application area scientists in the development of a new set of scientific simulation codes that can fully exploit our rapidly expanding computing resources. We will also spearhead state-of-the-art computing initiatives to develop architectures, applications, software systems, and test beds for petaflops-scale computing.

#### **Goal 8: National Security**

Argonne will help enhance national security by delivering new technologies and threat analyses for DHS, the Department of Defense, and the U.S. intelligence community. Many Laboratory discoveries and inventions developed in pursuit of our mission are now helping to increase homeland security. Notable technologies include portable systems for detection and field identification of concealed nuclear materials, pathogenic microorganisms, and airborne poisonous chemicals; models to guide infrastructure assurance; and the PROTECT system, which combines detection, communication, and quick-response strategies to protect subways and other enclosed public spaces against chemical and, eventually, biological attacks. Argonne is also exploring the sociological dimensions of terrorist threats by partnering with leading social scientists at the University of Chicago.

#### **Goal 9: Environmental Research**

Argonne will provide leadership in key areas of environmental research by integrating fundamental research with reliable impact assessments and innovative technological solutions. We will make major contributions in such areas as the cycling and sequestration of carbon, the causes and consequences of global climate change, atomic-level controls for contaminant sequestration, and potential environmental impacts of a hydrogen fuel economy. This research will take full advantage of the APS and other state-of-the-art facilities and tools available at the Laboratory.

#### **Goal 10: National User Facilities**

Argonne is committed to maximizing the scientific and technical productivity of its existing user facilities, especially its four leading national user facilities: the APS and IPNS (discussed above), the Argonne Tandem-Linac Accelerator System (ATLAS, which would become part of RIA), and the Electron Microscopy Center. Meeting this goal involves maintaining the facilities' high reliability and availability while increasing their performance and experimental capabilities. At the APS, for example, we plan

upgrades over the next two decades that will increase the facility's capabilities and users' productivity through a 1,000- to 10,000-fold increase in beam brightness. The benefit will be much more information, obtained much more quickly, to support such important scientific activities as imaging nanoscale devices and solving the atomic structures of the huge biological molecules crucial to understanding diseases. Argonne will remain an international leader in accelerator-based user facilities, through the APS, RIA, connections with high-energy and nuclear physics, and involvement in development of the next generation of x-ray sources after the APS.

### C. Scientific and Technical Core Competencies

To achieve our vision, we cultivate distinctive, world-class scientific and technical capabilities and integrate them into a dynamic portfolio of core competencies that serve and anticipate current and emerging national R&D needs in our mission areas. Our current competency portfolio includes the following:

- A complete set of engineering and scientific expertise supporting the design, development, and evaluation of current and advanced nuclear energy systems and proliferation-resistant nuclear fuel cycle technologies, including pyroprocessing.
- Design, construction, and operation of accelerator-based user facilities, along with diverse state-of-the-art capabilities related to acceleration, particle detection, synchrotron radiation techniques, spallation neutron scattering techniques, and the control and manipulation of particle beams and photon beams.
- Fundamental science and engineering expertise in, and at the interfaces between,
  - Materials sciences, chemical sciences, biological sciences, and atomic physics;
  - High-energy and nuclear physics;
  - Multidisciplinary nanoscience and nanotechnology;

- Structural biology, functional genomics, and bioinformatics;
- Environmental science and technology;
- Applied mathematics and computer science, including collaborative and virtual environments; and
- Computational science, including modeling, simulation, systems analysis, and complex adaptive systems.

Our goal in managing our portfolio of core competencies is to be best in the world in selected areas, to be among the leaders in other areas, and to have sufficient breadth and balance to both support users of the facilities we steward and tackle complex multidisciplinary challenges in our mission areas — typically in collaboration or partnership with others.

### D. Roles in Accomplishing DOE Missions

Argonne has a contractual responsibility to serve DOE's mission areas, especially its overarching national security mission. In *science* and in *energy*, we have a principal role. Our role in *environmental quality* is as a major contributor. Developments after September 11, 2001, demonstrated how fundamentally our knowledge, technologies, and facilities — even those originally developed for other purposes — serve as a major resource for *national security*.

#### 1. National Security

The recent evolution of threats to U.S. national security has amplified and focused our involvement in DOE's national security mission. Our contributions draw particularly on substantial Laboratory expertise in the nuclear fuel cycle, in chemistry and biology, and in systems analysis and modeling, along with the diverse enabling technologies and sciences underpinning those areas. We also have specialized R&D capabilities contributing to the development of new technologies for detection and attribution, such as highly sensitive instruments and verification technologies to detect radiation and chemical

threats or provide biological clues to possible weapons proliferation or actual attacks. Our skills in modeling and decision science are contributing to the security of critical infrastructure at local, regional, national, and global scales. In addition to this scientific and technical expertise, we have experience with other nations in cooperative R&D that will be valuable in supporting DOE goals relating to nonproliferation cooperation, export controls, and materials protection.

Scientific, engineering, and operational capabilities that we have developed over many years for other purposes are more recently yielding results that help to counter the threats of terrorism. In the future, our expertise, facilities, and technologies promise to address a broader range of important goals in national security and homeland defense, across the full spectrum of concerns about threat anticipation, threat mitigation, response, and recovery.

## 2. Science

For DOE's science mission, we operate major scientific user facilities and have significant experimental and theoretical research programs in nuclear and high-energy physics; in applied mathematics; and in materials, chemical, computer, computational, biological, environmental, and fusion science. In several key fields and subfields important to DOE, our research is among the most cited, and our scientists are international leaders. We take pride in effective collaborations with other DOE laboratories, strong interactions with the academic community, productive R&D partnerships with private industry, and high-quality research experiences provided for hundreds of undergraduate and graduate students each year.

The APS, IPNS, and ATLAS are among DOE's most successful major national scientific user facilities. The APS, the nation's premier hard x-ray synchrotron radiation facility, now serves nearly 5,000 users from universities, corporations, and national laboratories throughout the country, and it routinely reports newsworthy new science. The IPNS continues to provide extraordinarily reliable neutron beams and user support for approximately 400 experiments, while continuing its tradition of leadership in the development of

spallation targets, neutron moderators, and neutron scattering instruments. In addition to operating the APS and IPNS, we educate the next generation of users by hosting the National School for Neutron and X-ray Scattering. At ATLAS, unique low-energy heavy-ion beams enable over 100 scientists each year to conduct forefront research in nuclear, atomic, and applied physics. The RIA initiative — recently identified by the nuclear physics community as its highest priority among major new construction projects — derives considerable scientific motivation and much of its technology base from ATLAS.

For several years we have made significant contributions to major subprojects associated with user facilities or detectors located elsewhere. The most visible current example is our participation in the Spallation Neutron Source (SNS). We have lead responsibility for SNS spectrometer systems, and we provide substantial technical support for SNS target systems. Other examples include contributions to the ATLAS detector for the Large Hadron Collider, participation in the Linac Coherent Light Source, and detector fabrication for the MINOS neutrino experiment.

Science at Argonne benefits from access to major facilities and from the Laboratory's integrated approach to complex problems. The grand challenges in modern science, such as nanoscale materials or fundamental understanding of biological processes at the molecular scale, are beyond the reach of isolated experiments. Success requires not only forefront capability but also a suite of experimental and theoretical approaches. Our strength comes from diverse scientific teams that examine a problem from many complementary perspectives. This synergy of many approaches working together generates remarkable scientific power and often leads to the creation of pathbreaking new research facilities. The APS, IPNS, and ATLAS all had their origins in Argonne science.

Four of the major Laboratory initiatives featured in Chapter III of this *Institutional Plan* build on Argonne strengths that serve DOE's science mission, both through performance of forefront research and through service to users. Those four initiatives are the Center for Nanoscale Materials, the Rare Isotope Accelerator, Functional Genomics, and Petaflops Computing

and Computational Science. In addition, major components of the initiative Hydrogen Research and Development fall under DOE's science mission.

### 3. Energy

For its energy mission, Argonne serves with the Idaho National Engineering and Environmental Laboratory as co-lead laboratory for nuclear reactor technology. In addition, we have substantial programs and facilities serving DOE's mission to develop innovative, energy-efficient, cost-effective, and environmentally friendly technologies for electric power, transportation, and industry. Since the 1970s we have cultivated capabilities and programs — and have produced results — that are well aligned with recommendations of the administration's energy policy, as described in the May 2001 *Report of the National Energy Policy Development (NEPD) Group*. We operate numerous unique energy R&D facilities that are used by researchers from universities and industry.

We have noteworthy expertise and facilities in nuclear reactors, non-reactor nuclear facilities, and nuclear fuel cycle technologies. Over the years, we have developed safe and reliable fast-reactor technologies and have demonstrated the technical basis for a proliferation-resistant closed nuclear fuel cycle, based on pyroprocessing, that can consume weapons-grade plutonium and spent fuel from the nation's current fleet of power reactors. We are ready to contribute solutions that will allow nuclear energy to be a significant component of the nation's energy supply portfolio in both the near and long terms — safe, environmentally acceptable, proliferation-resistant, sustainable, and economical. The major Laboratory initiative Advanced Nuclear Energy Systems envisions a closed, environmentally sound nuclear fuel cycle that generates electricity — and possibly hydrogen — while reducing inventories of plutonium and the long-term toxicity of the waste generated. We played the key technical role in DOE's development of an R&D road map for "Generation IV" nuclear reactors and the Nuclear Hydrogen Initiative, and we are now conducting the R&D. We have the capability to contribute importantly to Generation IV

technologies, including reactors designed for some combination of electricity generation, waste management, and hydrogen production.

Our broader energy R&D portfolio is built on expertise in superconductivity, fuel cells, batteries, fossil fuels and carbon management, renewable energy technologies, energy testing and analysis, and other key technologies. Transportation technology R&D relies on many of these competencies and on unique Laboratory facilities to support DOE's quest to increase the efficiency and productivity of vehicular energy use while limiting environmental impacts.

The breadth of our R&D portfolio in both energy technology and supporting basic science is reflected in the range of contributions that we propose to make in support of the nation's new national hydrogen economy initiative. Our major Laboratory initiative in Hydrogen Research and Development encompasses extensive work on the materials science and chemistry of high-performance structural materials and catalysts, bolstered by use of the APS, IPNS, and other major research facilities; investigation of the production of hydrogen from nuclear power, taking advantage of our extensive expertise in nuclear reactor technology; and exploration of effective systems for utilizing hydrogen in both transportation and stationary applications, capitalizing on experience and facilities developed in earlier partnerships with industrial firms.

### 4. Environmental Quality

In support of DOE's environmental quality mission, we develop innovative characterization and remediation tools and technologies, create advanced technologies that intrinsically produce little or no pollution and minimize waste generation, clean up land and facilities on the Argonne sites, and conduct thorough and objective environmental analyses. The focus of this work is shifting from effluent control technologies and associated regulation toward resource and waste management, site remediation, long-term stewardship, and global environmental issues. Our strength is our combination of capabilities in bioprocessing, ecology, modeling and measurement of environmental pathways, atmospheric

physics and chemistry, environmental assessment, and decision models.

Our work in the environmental quality areas ranges widely. We are responsible for operating all three Climate Research Facilities of DOE's Atmospheric Radiation Measurement Program. In other work, we are using the APS to pioneer synchrotron-based environmental tools that will deepen microscale understanding of environmental processes. The Laboratory also belongs to the EnviroCAT partnership, which will develop state-of-the-art APS beamlines designed to tackle a broad range of environmental science problems. Elsewhere, the U.S. Department of the Interior has tapped Argonne to develop the environmental impact statement for the Trans-Alaska Pipeline System.

### **5. Enabling the Mission through Excellence in Operations**

Built into all Argonne programs and support activities is a commitment to operational excellence, to exemplary relations with the public (especially neighbors near the Illinois and Idaho sites), and to development of the diverse science and engineering workforce needed to accomplish DOE missions and assure U.S. prosperity, security, and leadership into the future. In the operations area, our contractual goal is to conduct all work and operate all facilities cost-effectively and with distinction, in a manner that integrates with and supports our missions in science, technology, energy, and environment, while fully protecting workers, facility users, the public, the environment, and national interests.

For most of the past half century, the University of Chicago has, as a public service, managed and operated Argonne under contract to the federal government. As a result, the Laboratory's research environment and performance have maintained a high standard of intellectual excellence and integrity, and the site — despite its age — is among the best maintained in the DOE complex. Currently, the University and the Laboratory are strengthening ties at all levels, from student research to joint appointments, collaborations between individual investigators, and strategic alliances.

### **E. Strategic Context and Planning Assumptions**

Argonne is one of DOE's nine major multiprogram national laboratories, and it is one of ten facilities affiliated with DOE's Office of Science. Like most DOE R&D sites, Argonne is managed and operated by a contractor. We serve all four of DOE's mission areas, and we are internationally recognized for our science, scientific user facilities, and energy R&D. Our track record of performance, our human resources, and our R&D facilities are the assets upon which the Laboratory's strategic plan for the future is built.

Our planning is based on five key assumptions:

- DOE's national laboratories must act increasingly as a synergistic system, with the laboratories managing their collective competencies, increasing their overall cost-effectiveness, and partnering on major initiatives among themselves and with the private and academic sectors.
- Sponsors, regulators, and the public will continue to require that we demonstrate responsible corporate citizenship. This imperative includes being a good and trustworthy neighbor, conducting operations cost-effectively and responsibly, and meeting or exceeding regulatory requirements.
- Argonne must compete on its merits for federal funding, for the "best and brightest" employees, and for the modern infrastructure needed for future success. Important factors in this competition will be scientific and technological excellence, cost-effectiveness, mission contributions, record of performance, and a working environment that enables high performance from a diverse and talented workforce.
- Robust links with universities, industry, federal laboratories, and the general scientific and technical community (within the United States and abroad) are essential if we are to maintain our leadership and fully exploit advances made throughout the world.
- Computing, computational science, and communications and information technology

will advance rapidly, will become seamlessly intertwined with experimental science, and will thereby revolutionize many fields of research and applications that are central to the missions of DOE and Argonne.

## F. Strategic Objectives

*Objective 1. We will continue to perform outstanding science and technology consistent with our mission and will provide results and value to the nation. This objective includes operating world-class scientific user facilities and providing other science- and technology-based tools in a way that maximizes service to users and research productivity, as well as other public benefits.* Outstanding science and technology are Argonne's *raison d'être*. The Laboratory's history of accomplishment is the basis on which it becomes the performer of choice in its mission areas. In support of this objective, we expand the frontiers of knowledge, develop and test new technologies, and create new areas of inquiry that keep us at the forefront. Thousands of scientists and students from universities, industry, and other laboratories around the country and the world use our unique facilities to conduct their research. Reliable facility operation, meeting or exceeding performance specifications, and high-quality user support are critical. In addition to the APS, IPNS, and ATLAS, we operate or provide other important special research tools, such as major nuclear research facilities, environmental research sites, mathematical libraries, software packages, and decision tools.

We have an obligation to the taxpayer to provide the highest possible mission value with the resources we receive. Under constrained or declining budgets, this goal can be achieved only by nurturing the best, most important programs and phasing out the least important. Only by making such choices can we ensure that the research we undertake achieves the required quality and stature. In the near term, we will emphasize expanding and strengthening the computational components of our R&D; operating user facilities effectively; operating and improving reactors and other nuclear facilities; expanding capabilities for research on nuclear fuel cycle technology; providing radioisotope power sources

and developing advanced nuclear energy sources for space exploration and national security; applying diverse expertise to homeland security; exploring promising areas at the interfaces between traditional disciplines; solving problems of national importance; and catalyzing the expeditious transfer of our technologies into beneficial use. Chapter IV provides updated plans for each of our major science and technology areas.

*Objective 2. We will develop important new R&D initiatives and scientific facilities that serve emerging national needs consistent with our mission and will implement them cost-effectively and expeditiously to the benefit of DOE and the nation.* New initiatives are an engine for change. They attract bright research staff and facility users, and they help direct our programmatic focus onto current and future needs. Each year we feature a few major Laboratory initiatives that promise extraordinary, broad benefits and that build naturally on our mission areas and strengths. This year's portfolio includes the Center for Nanoscale Materials, the Rare Isotope Accelerator, Functional Genomics, Petaflops Computing and Computational Science, Advanced Nuclear Fuel Cycle, and Hydrogen Research and Development. Chapter III summarizes these major Laboratory initiatives.

*Objective 3. Argonne and the University of Chicago will strengthen and fully exploit partnerships and alliances to maximize the Laboratory's value and impact — nationally, regionally, and locally.* A strong intellectual alliance between the University of Chicago — one of the nation's premier research universities — and Argonne — one of DOE's major multiprogram science laboratories — promises benefits to DOE and to the broadly ranging impacts of both institutions. Argonne and the University are increasingly taking advantage of each other's complementary expertise in areas such as nanoscience, computing and computational science, bioscience, environmental science, homeland security, and economic modeling of energy systems. The two institutions plan to increase joint recruiting, joint proposals, joint appointments, joint projects, and sharing of facilities and other resources.

*Objective 4. The University of Chicago and Argonne will continuously improve the*

*cost-effectiveness, management, and operations of the Laboratory.* The University of Chicago is working with DOE to continuously improve and streamline Argonne's administration and operation. Major challenges include recruiting and developing a diverse workforce, modernizing the physical infrastructure, and fully exploiting partnerships. The changes undertaken in this quest will build on best practices gleaned from the private, academic, and public sectors. The result

will be an integrated, creative, and high-performing laboratory whose performance significantly exceeds the sum of its parts, because it engages — productively, cost-effectively, safely, securely, and environmentally responsibly — as a contributing member of the DOE laboratory system and as a partner and leader in addressing national needs in science and technology. Chapter V in this *Institutional Plan* describes our status and plans in operations areas.



# III. Major Laboratory Initiatives

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This chapter provides planning “snapshots” of Argonne’s major Laboratory research initiatives, for consideration by DOE.<sup>1</sup> These initiatives represent important opportunities to enhance U.S. research capabilities, to serve the broader scientific community, and to advance scientific understanding and engineering achievement across a wide range of disciplines. They lie at the heart of many of the Laboratory’s *strategic goals*, as introduced in Chapter II.

Argonne carefully considers the implications of the National Environmental Policy Act (NEPA) for its scientific and technical initiatives, as early as it is reasonable to do so. For initiatives where NEPA implications are expected to be significant, the implications will be discussed explicitly in this *Institutional Plan*.

The six major Argonne initiatives relate most closely to two DOE mission areas, Science and Energy:

- Science
  - Nanosciences and Nanotechnology — Center for Nanoscale Materials
  - Rare Isotope Accelerator
  - Functional Genomics
  - Petaflops Computing and Computational Science
- Energy
  - Advanced Nuclear Energy Systems
  - Hydrogen Research and Development

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<sup>1</sup> Inclusion of initiatives in this chapter does not necessarily imply approval, or an intention to implement, by DOE. All funds received for initiatives during FY 2004 are included in the resource tables in Chapter VI of this *Institutional Plan*. However, resources required for proposed growth of initiatives in years beyond FY 2004 are generally not included in those projections. Projected resource requirements for all initiatives include costs associated with protection of the environment and the health and safety of workers and the public.

In addition to these six major Laboratory initiatives, we are applying our capabilities to national security. In the next chapter, Section IV.C explains these efforts and presents five programmatic initiatives in the areas of nuclear national security and homeland security. These initiatives point toward more extensive future program development in support of DOE’s core national security mission, from which flow all of the Department’s missions.

## A. Science

### 1. Nanosciences and Nanotechnology — Center for Nanoscale Materials

Argonne’s Center for Nanoscale Materials (CNM) was approved in FY 2002 as one of five such centers created by DOE to support the National Nanotechnology Initiative. This interagency initiative is driven by the realization that the emerging field of nanoscience shows extraordinary promise for overcoming the scientific and technological limits of present-day materials and processes.

Argonne’s vision is to create new nanoscale materials as the basis for future technologies. Highlights of our plan include focusing on chemical methods to self-assemble nanostructures, to pattern nontraditional electronic materials, and to create new probes for exploring nanoscale phenomena. We also aspire to help pioneer the new fields of molecular and magnetic electronics, lay the foundations for new chemical and biological sensor technologies, and develop novel nanomaterials for energy applications.

The CNM’s nanoscience and nanotechnology research will grow out of Argonne’s existing core competencies in materials science, chemistry, biology, and computing and our advanced characterization capabilities at the Laboratory’s Advanced Photon Source (APS), Intense Pulsed Neutron Source (IPNS), and Electron Microscopy Center. Our objective is to create a

multidisciplinary research environment that fosters collaboration across the Laboratory's and the University of Chicago's many divisions and departments. Emerging CNM research directions include bio-inspired materials, nanomagnetism, nanocarbon, and nanoscale phenomena in oxide materials.

The CNM will serve as a forefront research center and a user facility for regional and national research communities. Until now, DOE's major materials science user facilities — such as the APS and IPNS — have focused mainly on materials characterization. In contrast, the CNM is a new-generation user facility with the primary goal of fabricating advanced nanoscale materials. The CNM will complement and enhance Argonne's other user facilities by creating cutting-edge nanomaterials that require advanced characterization. To maximize this synergy, the CNM's new building will adjoin the APS, where the CNM will construct a state-of-the-art, hard-x-ray nanoprobe beamline. The new beamline will focus hard (10-keV) x-rays down to an unprecedented spot size of 30 nanometers, enabling a wide variety of imaging, spectroscopic, and diffraction experiments that cannot be performed anywhere else in the world.

Solid-state electronics has been a key driver of economic growth since the middle of the 20th century. In the 21st century, researchers will expand this technology by creating connections between biological and nonbiological materials. The CNM will create novel interconnections between soft matter, such as complex organic and biological molecules, and hard matter, such as solid-state nanoparticles and patterned systems. Major phenomena of interest will include the flow of chemical energy and the propagation of light. Our work in these areas recently received competitive funding from the Nanoscale Science, Engineering, and Technology program in DOE's Office of Basic Energy Sciences (DOE-BES).

Our research in nanomagnetism focuses on creating new nanostructures by using chemical self-assembly and lithographic patterning of thin-film hybrid systems. Use of the spin (magnetism) of the electron, in addition to its charge, is opening the new field of magnetic electronics, known as "spintronics." The CNM will investigate spintronics, along with molecular electronics and

nanophotonics, to develop new functionalities at the nanoscale.

We will also explore bio-inspired composites as a path to creating new materials with entirely new functions. The electronic and optical properties of inorganic materials and the exquisite molecular recognition and reaction specificity of organics will allow us to create novel composites with wide-ranging applications. Examples include *in vivo* gene surgery; hydrogen production, storage, and catalysis; self-assembled molecular electronics circuits; and advanced biosensors. A recent success is the discovery of a method that uses novel hybrid, nanometer-sized metal-oxide semiconductors to control and initiate chemical reactions of DNA. The CNM's research on bio-inspired composites leverages Argonne's expertise in semiconductor and metal nanoparticle synthesis, nanocrystalline diamond, ferroelectrics, and chemical synthetic processes.

An emerging topic of high interest for the CNM is the role of theory in creating computational algorithms that simulate nanoscale phenomena. Multiple approaches will be needed to simulate and model complex materials phenomena ranging from self-assembly in inorganic and biological systems to electronic, photonic, or thermal transport on the nanoscale. CNM research will lead efforts to develop multi-scale theories that leverage Argonne's petaflops computing initiative (see Section III.A.4); our Materials Theory Institute (which hosts visiting theorists studying condensed matter); and the forefront theory capabilities of the Laboratory and the University of Chicago in chemistry, materials science, and biology. Within the CNM, the Virtual Fab Lab will develop computational algorithms for simulating the behavior of nanoscale systems, enabling the virtual fabrication and testing of new devices. In August 2003 the Virtual Fab Lab held a workshop that brought together more than 50 prominent scientists from the national computational nanoscience community and from CNM research theme areas. This workshop focused on grand challenges in modeling the assembly and properties of nanomaterials.

The CNM will energize new collaborations and partnerships that broaden its user community throughout the Midwest and the nation. To foster the user community and stimulate feedback from

users, we and our partners have held general and specialized workshops, and more are planned. Research themes already covered include the x-ray nanoprobe, neutrons and nanoscience, and industrial microfabrication. Under the aegis of the University of Chicago-Argonne Consortium for Nanoscience Research, which was launched in 2001, investigators from the two institutions are cooperating to pursue initial research themes that embrace major CNM focus areas. The investigators also have begun ambitious planning for intellectual cross-pollination and educational outreach.

Planning for the CNM infrastructure is well under way. The state of Illinois has committed funds for the CNM building. Design of the building by the architectural and engineering firm M.W. Zander is complete, and construction has begun. Jacob Facilities, Inc., is the construction management firm.

The CNM initiative requires investments in the following three areas:

1. *Personnel.* Our current staff already includes some of the researchers required for this initiative, and several of our core programs will naturally move in directions that complement the CNM. In addition, many new staff members with special expertise will be recruited in such areas as self-assembly, lithography, advanced spectroscopies, and imaging. Creation of the Virtual Fab Lab will require critical new staff with expertise in theory and computational nanoscience.
2. *New Tools for Nanofabrication.* Electron lithography and focused-ion-beam lithography are essential tools for nanostructure fabrication. Equipment will also be required for etching, deposition, and other processes. Several of these tools will strongly attract outside users to the CNM, because the tools are currently unavailable in the Midwest. Clean rooms and related infrastructure must be developed to provide the scrupulously clean conditions required for the fabrication of nanostructures that are much smaller than a speck of dust.
3. *New Tools for Nanocharacterization.* Tools for visualizing nanostructures — especially x-ray, electron, scanning probe, and

near-field optical microscopes — will be developed further at Argonne. At the APS, the x-ray nanoprobe will be developed to exploit the facility’s brilliant beams for studies of materials at the nanoscale. The productivity of our Electron Microscopy Center (see Section IV.A.2) will be enhanced by synergies with the CNM, and the IPNS will attract new users to characterize the new materials created at the CNM.

Resources required for this initiative are summarized in Table III.1. We are working with the state of Illinois to build the CNM building by January 2006. Funding for instrumentation and research operations is being provided by DOE-BES (KC-02 and KC-03), the state of Illinois, and other sources.

**Table III.1 Nanosciences and Nanotechnology — Center for Nanoscale Materials** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs							
Operating <sup>a</sup>	1.5	1.5	4.8	18.5	19.0	19.5	20.0
Capital Equipment	10.0	12.0	14.0	-	-	-	-
State Grant <sup>b</sup>	17.0	-	-	-	-	-	-
Total	28.5	13.5	18.8	18.5	19.0	19.5	20.0
Direct Personnel	5.0	15.0	22.0	60.0	62.0	65.0	67.0

<sup>a</sup> Not included here is funding for in-house nanoscience research, for which Argonne will compete separately. The magnitude of this additional funding is expected to be similar to that of the initiative’s operating funding.

<sup>b</sup> The indicated grant funding from the state of Illinois is for construction of a CNM building. In FY03, \$19 million was received.

**2. Rare Isotope Accelerator**

In November 2003 DOE’s Office of Science (DOE-SC) published *Facilities for the Future of Science: A Twenty-Year Outlook*, which assigned the highest priority among proposed large-scale research facilities to the Rare Isotope Accelerator (RIA). When completed, RIA will provide researchers with accelerated beams of extremely short-lived radioactive elements — “rare isotopes” — and will make possible cutting-edge research in the fundamental sciences of nuclear physics and nuclear astrophysics.

Our present understanding of atomic nuclei does not allow us to reliably predict the properties of nuclei with unusual ratios of protons to neutrons. Yet these nuclei hold the keys to unlocking fundamental questions about the nature and history of matter and the cosmos. RIA will enable researchers to determine the properties and structure of these nuclei and to answer such fundamental scientific questions as these:

- How are the properties of short-lived atomic nuclei derived from the interactions among their constituents?
- How are the heavy elements created?
- How do the heavy elements' nuclear properties influence stars?
- Why do complex nuclei exhibit simple symmetries?
- What are the fundamental symmetries of nature, and how can rare isotopes help us investigate them?

In addition, research at RIA is expected to create new applications in materials science, biology, and medicine, and to play an important national security role in the science-based stockpile stewardship program.

These compelling scientific opportunities led the DOE-National Science Foundation (NSF) Nuclear Science Advisory Committee (NSAC) in its *2002 Long Range Plan for Nuclear Science* to recommend RIA as the field's highest priority for major new construction and to conclude that RIA is required to ensure U.S. leadership in the areas of nuclear structure and nuclear astrophysics. The NSAC recommendation is reflected in the recent DOE-SC strategic plan for major construction projects. Other support for RIA growing out of discussions in scientific forums in the United States and abroad includes a 1999 recommendation from the National Research Council's Committee on Nuclear Physics. More recently, the National Science and Technology Council's 2004 report, *A 21st Century Frontier of Discovery: The Physics of the Universe*, recommended that DOE and the NSF "generate a scientific roadmap for the proposed Rare Isotope Accelerator in the context of existing and planned nuclear physics facilities worldwide."

Following DOE's approval of mission need in February 2004, the RIA project began preparations for the site selection competition. This competition will help clarify the conceptual design and move forward with preliminary design.

Recognizing that exploration of the scientific frontier will require extensions of today's technical capabilities and facilities, Argonne has developed a concept to achieve the physics goals set forth for RIA by NSAC and the scientific community. In work on the RIA project, we collaborate with other U.S. research institutions. Technology development for RIA is under way at ten institutions, including universities and national laboratories. We are working with the research community to organize the RIA team and prepare a pre-conceptual design report, an expected requirement for the site selection process.

Our concept for RIA is based on two accelerators: a primary heavy-ion driver linac, based on technology developed at Argonne and Jefferson Lab (elements of which are currently being used for the Spallation Neutron Source), and a second accelerator, based on Argonne's existing state-of-the-art heavy-ion accelerator, ATLAS (Argonne Tandem-Linac Accelerator System). In our plan, the second accelerator will be located downstream of the rare isotope production target to focus and reaccelerate isotope beams to the experimental areas. Because the ATLAS technology can accelerate any element from hydrogen to uranium, a variety of mechanisms can be used to optimize rare isotope production. ATLAS also has excellent transverse and longitudinal phase space properties, and it excels in beam transmission and timing characteristics. These capabilities are important for nuclear structure investigations and astrophysics experiments, where the beam quality requirements are especially stringent.

In the past year, we have achieved significant technical advances demonstrating the following key elements of our RIA design:

1. Construction of a full-scale RIA gas-stopping cell and tests demonstrating the required ion extraction efficiency.
2. Operation of a half-scale, windowless, flowing-liquid lithium target at the beam power deposition energy anticipated for RIA.

This target will serve as the prototype for heavy-ion fragmentation targets.

3. Construction and testing of three new classes of intermediate-velocity superconducting accelerating cavities to validate current baseline technology assumptions.
4. Detailed simulations of beam dynamics and beam loss for the entire driver accelerator.

Preliminary estimates of effort, time lines, and cost suggest that this major new facility can be built at Argonne within DOE’s planning window, following approximately two years of detailed facility design.

Funding for RIA (Table III.2) is being sought from the Nuclear Physics (KB-04) program. A major challenge is to increase DOE’s total nuclear physics budget sufficiently to allow RIA to proceed. Argonne’s plan for RIA calls for substantial completion of capital construction in 2011, with commissioning extending through 2013. This plan achieves the objectives of the RIA project while recognizing the need of DOE-SC to set priorities across its full portfolio of prospective major construction projects.

**3. Functional Genomics**

The biological sciences now stand at the threshold of developing new conceptual structures — facilitated by informatics and large-scale computation — that will transform biology from an almost exclusively experimental science to one in which theory plays a key role. Recent developments in DNA sequencing, analytical tools, and computing technology have made it feasible to construct a complete map of cellular function.

The comprehensive understanding of biomolecular function has huge potential payoffs, including new strategies for altering cellular activities and creating new cellular capabilities. These opportunities can lead to solutions for problems associated with the DOE science mission and will be particularly important for advancing the DOE national security mission through the study of organisms used as biowarfare agents. More broadly, the resulting advances will provide major benefits for environmental management, human health, and general economic productivity.

Despite the benefits of mapping cellular functions, the scientific challenges are significant. Success will require substantial enhancement of existing experimental and computational capabilities. A comprehensive understanding of even the simplest single-cell organism requires the functional analysis of thousands of proteins and other macromolecules. The amount of data needed for this task greatly exceeds that required to sequence the genome. Furthermore, compared to genome sequencing, functional analysis requires novel computational approaches and experimental technologies with faster throughput rates.

To help seize these opportunities, Argonne is continuing a major initiative to undertake the large-scale, functional characterization of genomes, which will advance the goals of DOE’s Genomes to Life program. Our Functional Genomics initiative comprises three components: (1) structural genomics, (2) high-throughput molecular biology and biochemistry, and (3) bioinformatics. The facilities developed for this initiative will serve the entire research community by providing researchers from universities and industry with a broad range of

**Table III.2 Rare Isotope Accelerator** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10	FY11	FY12	FY13	FY14
<b>Costs</b>											
Operating	6.0	15.0	20.0	37.0	39.0	38.0	25.0	55.0	75.0	75.0	80.0
Capital Equipment	-	-	-	-	-	-	-	-	-	-	-
Construction	-	-	-	16.0	27.0	98.0	175.0	145.0	125.0	73.5	-
<b>Total</b>	<b>6.0</b>	<b>15.0</b>	<b>20.0</b>	<b>53.0</b>	<b>66.0</b>	<b>136.0</b>	<b>200.0</b>	<b>200.0</b>	<b>200.0</b>	<b>148.5</b>	<b>80.0</b>
<b>Direct Personnel</b>	<b>15.0</b>	<b>40.0</b>	<b>50.0</b>	<b>120.0</b>	<b>140.0</b>	<b>235.0</b>	<b>310.0</b>	<b>360.0</b>	<b>390.0</b>	<b>320.0</b>	<b>260.0</b>

capabilities needed to study molecular processes in the cell.

The *structural genomics* component of this initiative will evolve from our Structural Biology Center (SBC) — one of the world's best facilities for collecting high-resolution data from crystals of macromolecules and macromolecular complexes. Meeting the crystallographic needs of this initiative will require greater throughput at the SBC, which we plan to achieve by enhancing existing detectors and upgrading optics and robotics capabilities.

The initiative's structural genomics component also involves high-throughput production and crystallization of proteins. The Midwest Center for Structural Genomics (MCSG), funded by the National Institutes of Health (NIH), has developed robotic facilities for protein cloning, expression, and purification. Significant expansion of these facilities will be required to achieve this initiative's goals. To house facilities for high-throughput protein crystallization, we have proposed that the state of Illinois fund construction of a new facility, the Advanced Protein Crystallization Facility, to provide more than 40,000 square feet of laboratory space.

The *high-throughput molecular biology and biochemistry* component of this initiative will develop through the growth of facilities, capabilities, and expertise originally developed for the MCSG. Critical to this growth will be the development of capabilities to produce and characterize proteins and affinity reagents. Affinity reagents are antibody-like molecules that bind to specific proteins, making possible a wide range of biochemical and biological experiments to determine protein function.

In partnership with Los Alamos National Laboratory, we are preparing a proposal to DOE for the construction of a major Protein Production and Characterization Facility. Our goal is to produce all the proteins that make up the genome, as well as the reagents needed for high-throughput functional characterization. This facility will seek to establish a new standard for biochemical and biophysical characterization of proteins.

The initiative's *bioinformatics* component will encompass computational structural biology and will develop novel databases of genomes and

proteomes (the collections of proteins found in particular cell types) to support high-throughput experiments. A significant challenge will be to integrate the massive amounts of data from the Functional Genomics initiative with the vast quantities accumulating in public databases around the world.

We have sought input throughout the research community on strategies and procedures for this initiative. In September 2001 we hosted a workshop on the challenges of integrating genome and proteome databases. Since then, we have hosted three additional workshops on protein production and characterization. A fourth workshop is planned on proteomic data standards.

Our efforts in functional genomics will take advantage of a number of important existing resources at Argonne and the University of Chicago. The SBC at the APS will be key for producing high-resolution images of gene products. Such images are the best way to link the sequence information generated by genome projects to the functional data from our Functional Genomics initiative. The APS and the IPNS will be used for small-angle scattering studies of macromolecular complexes (molecular machines). These complexes will be identified by protein-protein interaction mapping and generated in high-throughput protein production facilities. Protein chips for studying protein-protein interactions will be developed in cooperation with our biochip program (see Section IV.B.6). Gene expression studies will be carried out in partnership with biochip facilities at the University of Chicago. Finally, our computer scientists will create a computational environment for information management and for analysis and integration of functional data. Computer simulations are essential to the development of systems biology capabilities; our Functional Genomics initiative will include a major simulation effort focused on the systems biology of prokaryotes (single-celled organisms without nuclei).

To develop comprehensive functional information on whole organisms, we will enhance our existing protein production capabilities. At the same time, we will establish new facilities for (1) high-throughput mapping of protein-protein interactions; (2) identification of high-affinity, high-specificity ligands for all gene products; and

(3) biochemical and biophysical characterization of protein function (e.g., enzyme assays).

We will partner with the University of Chicago to develop state-of-the-art, intermediate-voltage cryoelectron microscopy and associated image-processing capabilities.

Our Functional Genomics initiative is designed to advance the goals of the Genomes to Life program of DOE's Office of Biological and Environmental Research (DOE-BER). The four goals of this program are to (1) identify and characterize the molecular machines of life, (2) characterize gene regulatory networks, (3) characterize the functional repertoire of complex microbial communities in their natural environments at the molecular level, and (4) develop the conceptual framework and the computational capabilities needed to advance understanding of complex biological systems and predict their behavior. Key to this program is a systems biology approach to understanding how molecular machines and other cellular components function together in a living system. Developing capabilities for comprehensive functional characterization of entire genomes is critical to the program's success.

Elements of our Functional Genomics initiative are expected to attract sponsorship from NIH. Table III.3 describes the overall resources required, including the efforts of computer scientists, environmental scientists, and APS staff, as well as biologists working in the areas of structural and functional genomics. The increase in resources leading up to FY 2005 reflects anticipated expansion of computational and robotics capabilities, as well as NIH funding to support sector development and operation for an experimental station (the GM/CA-CAT) at the APS. These increases will support multiple Argonne research divisions working in the areas of computation, engineering, and molecular biology to determine the molecular structure and function of macromolecular complexes. DOE funding will be sought from DOE-BES (Energy Biosciences; KC-03) and from DOE-BER (KP-11), including the latter office's Genomes to Life program.

**Table III.3 Functional Genomics** (\$ in millions BA, personnel in FTE)<sup>a</sup>

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
<b>Costs</b>							
Operating <sup>b</sup>	14.3	16.5	17.7	18.6	19.5	20.5	21.5
Capital Equipment	-	1.3	1.3	1.6	1.6	1.6	1.6
Construction (state) <sup>c</sup>	-	1.5	10.0	22.0	-	-	-
Construction (DOE) <sup>d</sup>	-	5.0	30.0	55.0	40.0	16.0	-
Total	14.3	24.3	41.6	43.2	42.1	62.1	74.1
<b>Direct Personnel</b>	<b>55.2</b>	<b>69.3</b>	<b>73.4</b>	<b>75.4</b>	<b>77.4</b>	<b>79.4</b>	<b>81.4</b>

<sup>a</sup> Resource projections include funding from the National Institute of General Medical Sciences for the MCSG, plus anticipated funding from NIH, DOE-BER, and other organizations.

<sup>b</sup> Includes anticipated funding from NIH and the National Institute of General Medical Sciences for development of the GM/CA-CAT sector at the APS (enclosures, utilities, and undulators and other insertion devices).

<sup>c</sup> We have proposed that the state of Illinois fund construction of the Advanced Protein Crystallization Facility.

<sup>d</sup> Argonne's part of the Protein Production and Characterization Facility, being proposed to DOE.

#### 4. Petaflops Computing and Computational Science

Computer-based simulation continues to greatly advance scientific understanding of fundamental phenomena. In 2004 DOE's *Office of Science Strategic Plan* identified computational science as "increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering." Indeed, computation has become a third way of doing science, complementing — and in some cases, substituting for — the conventional methods of theory and experimentation.

In recognition of the critical importance of advanced computing, Argonne has established a Petaflops Computing and Computational Science initiative. The aim is to accelerate progress in computational science through an ambitious program comprising four major components: (1) a Laboratory-wide computational science program, (2) development of a national leadership computing facility, (3) a targeted R&D program, and (4) a new theory and computing sciences building.

In the spring of 2002 we initiated a Laboratory-wide computational science program

with the establishment of the *Laboratory Computing Resource Center*. The center's driving mission is to enable and promote computational science and engineering across Argonne, primarily by operating advanced computing facilities and supporting the use and development of applications. As a first step toward this goal, in late 2002 we deployed a 350-node teraflops-scale Linux cluster. To date, more than 50 Argonne projects involving 250 individual users are actively using this cluster. These projects represent a broad cross section of our competencies, including applied mathematics, biosciences, chemistry, climate research, computer science, engineering applications, environmental science, geology, nanoscience, nuclear engineering, and physics. The Linux cluster, in conjunction with our work in computational science, has enabled significant advances in many application areas. A notable example is nuclear energy, where we are developing simulation models under the Numerical Nuclear Reactor project (a joint effort with the Korean Atomic Energy Research Institute and part of the International Nuclear Energy Research Initiative). Building on these successes, we will next expand use of the cluster to new disciplines; make possible comprehensive scientific data management across the Laboratory; and improve the quality, performance, and scale of many computational applications at Argonne.

Our current cluster computer is the Laboratory's first terascale system. To solve today's most challenging scientific problems, however, will require ultrascale computers that take advantage of parallel multiprocessing. Since the early 1980s we have led efforts to acquire and evaluate the high-performance computers of the time. Our Advanced Computing Research Facility was one of the first facilities to make diverse parallel computers available to researchers for experimentation. In the late 1990s we were one of four sites designated a federal Advanced Computing Research test bed. Continuing this strong tradition, we now have begun working with Oak Ridge National Laboratory to formulate a vision for a *National Leadership Computing Facility*. This facility will deploy new "leadership-class" architectures for the high-end production computational simulation capabilities needed to meet national-scale scientific challenges. Ideally, in 2005 we will field a large (50-teraflop) IBM

BlueGene/L system that will enable a range of scientific experiments and serve as an initial platform for evaluating scalability for successor platforms. Planned subsequent increases in system size and performance will support sustained computational power of one petaflop ( $10^{15}$  operations per second) before the end of the decade.

In identifying key applications for our experiments in ultrascale computing, we have established a *targeted R&D program* focusing initially on two major areas: systems biology and nanoscience. DOE has identified both of these areas as critical, the former as part of the Genomes to Life program of DOE-BER and the latter as part of the National Nanotechnology Initiative. In collaboration with researchers at the University of Chicago, we are analyzing model organisms and designing a whole-cell modeling system. We have also begun to develop an integrated nanoscience simulation environment, a joint effort involving our Chemistry, Materials Science, and Mathematics and Computer Science Divisions. A common challenge in all these R&D areas is the need to devise new mathematics for modeling processes taking place on vastly different time and length scales.

Expansion of the Laboratory's computational science programs, as well as the addition of large-scale computers, has underscored the need for additional space. We are in the final stages of preparing for a *new theory and computing sciences building*, following more than a year of planning and discussion. Once final approvals are obtained, we estimate that construction can be completed within 18 months of groundbreaking. This state-of-the-art facility will include a large-scale computer room capable of housing the petaflops computing system we envision, and it will incorporate digital collaboration technologies to support distributed meetings and collaboratories.

Resources required for the Petaflops Computing and Computational Science initiative are specified in Table III.4. Included are costs for facilities and for a concomitant increase in personnel (systems staff, postdoctoral researchers, scientific programmers, and permanent research staff). Funding will be sought from the Mathematical, Information, and Computational Sciences Division (KJ-01) and from other sponsors within DOE-SC.

**Table III.4 Petaflops Computing and Computational Science** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs							
Operating	-	6.3	10.0	15.0	20.0	25.0	25.0
Capital Equipment	-	15.0	15.0	40.0	40.0	40.0	40.0
Construction <sup>a</sup>	-	-	3.7	3.7	3.7	3.7	3.7
Total	-	21.3	28.7	58.7	63.7	68.7	68.7
Direct Personnel	-	30.0	50.0	70.0	90.0	100.0	100.0

<sup>a</sup> Detailed planning for the advanced computation building will occur in FY04. Calculation of construction costs assumed third-party financing for FY04 and FY05, with leasing to begin in FY06. The calculated leasing and operations costs are based on 132,000 square feet at \$28 per square foot.

## B. Energy

### 1. Advanced Nuclear Energy Systems

The need to produce increasing amounts of energy and still reduce the resulting environmental burden dictates that nuclear power will play a major role in the world’s future portfolio of energy-production technologies. Large-scale expansion of nuclear energy cannot take place, however, until solutions are developed for the problems associated with spent fuel disposition and nuclear nonproliferation. The best way to address those two problems is through an advanced nuclear fuel cycle that returns fuel to the reactor and produces waste forms that are more benign.

The need for an advanced nuclear fuel cycle was recognized in the May 2001 report of the National Energy Policy Development Group, which stated that “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.” This need was recognized more recently in the May 2002 summit meeting between President Bush and Russian President Putin. Speaking for their governments, the two leaders agreed that advanced technologies for nuclear reactors and fuels hold promise for significant reduction in the volume of waste produced by civilian reactors, high proliferation resistance, and

decreased stocks of excess weapons-grade plutonium and other dangerous nuclear materials.

Argonne has been collaborating with DOE-Nuclear Energy, Science and Technology (DOE-NE) — as well as with other national laboratories, industry, and international partners — to formulate DOE’s Advanced Fuel Cycle Initiative (AFCI) and DOE’s program to develop the next generation of nuclear reactors (Generation IV Nuclear Energy Systems). The combined overall objective of the two DOE programs is to develop the base for a set of new, globally secure, sustainable nuclear technologies that (1) will allow nuclear power to become a publicly acceptable, growing part of the energy supply mix in the United States and abroad and (2) can compete in diverse markets with the most cost-effective alternative technologies. This technology set would also reduce and stabilize inventories of spent nuclear fuel, securely manage problematic nuclear materials, enhance proliferation resistance, and restore U.S. global leadership in nuclear technology.

In collaboration with international partners, DOE’s AFCI aims to develop and demonstrate these nuclear technologies and systems. The AFCI’s two key technologies and systems are (1) a closed, proliferation-resistant fuel cycle and (2) the Generation IV reactor technologies being pursued by DOE and the Generation IV International Forum. Argonne therefore proposes to develop and demonstrate (1) a fuel cycle based on advanced processing technologies and (2) Generation IV technologies based on fast-spectrum nuclear reactors.

In addition to having decades of experience in fast-reactor R&D, Argonne is a leader in developing advanced separation methods, based on both aqueous and pyroprocessing technologies, that can close the nuclear fuel cycle. As part of this initiative, we will assess both pyroprocessing and advanced aqueous options to determine their appropriate roles in meeting DOE’s AFCI objectives. Moreover, we plan to continue supporting the development of transmutation system models and assessing transmutation options, including transmutation in thermal reactors.

Argonne’s Advanced Nuclear Energy Systems initiative has five components that are mostly

coordinated with DOE's AFCI and its Generation IV Nuclear Energy Systems program: (1) nuclear systems (including transmutation) for advanced fuel cycles, (2) advanced separations technologies, (3) fuels for advanced nuclear systems, (4) advanced reactor technologies, and (5) a facility for treating spent fuel from light-water reactors.

*Nuclear Systems for Advanced Fuel Cycles.* Understanding the transmutation process in fast-neutron-spectrum reactors is important to the success and optimization of an advanced fuel cycle. A key goal of DOE's AFCI is to transmute long-lived actinides into shorter-lived elements to ease the burden of storing nuclear wastes in a geologic repository. Argonne proposes to improve the definition of key technical elements of a transmutation strategy and to perform R&D that resolves technical issues in transmutation strategies, enables comparison of options, and supports key decision making. The required activities, to be performed mostly at the Illinois site, include design of (1) thermal- and fast-reactor cores for transmutation and (2) the associated fuel cycle strategies. Both would be optimized to support DOE's AFCI objectives. Our current work on transmutation science focuses on informing near-term decisions about the fuel cycle and the implementation path for an advanced nuclear system. Physics experiments are needed to resolve key technical issues related to actinide transmutation in such advanced nuclear systems, in order to support the design of transmutation-related experiments and to analyze experimental results.

*Advanced Separations Technologies.* Argonne-East leads the development of advanced aqueous and pyroprocessing technologies, sharing work between the Illinois and Idaho sites. Both separations technologies are being developed to meet DOE's AFCI objectives, which aim for efficient, proliferation-resistant technologies that can support a transition to sustainable nuclear power production. Development of the aqueous technology will require optimizing flow sheets and demonstrating the process through laboratory- and engineering-scale testing. Pyroprocessing is currently used on a production scale at Argonne-West to treat spent fuel from the Experimental Breeder Reactor-II, but the technology needs further development for advanced closed fuel cycles. Pyroprocessing also holds promise for

treating spent fuel from light-water reactors, but first a front-end process must be developed to reduce oxide fuel to a metal form suitable for electrorefining. A process to recover plutonium and other transuranic actinides for recycling into fast-reactor fuel must also be developed and demonstrated. Integral to progress toward an advanced fuel cycle is the development of waste forms and associated storage technology. The metal and ceramic waste forms that result from pyroprocessing must be fully characterized and qualified for disposal in a repository.

*Fuels for Advanced Nuclear Systems.* Suitable advanced fuels need to be developed for Generation IV reactors, which will operate with different coolants and at higher temperatures than earlier reactors. Advanced fuels must be compatible with the coolant, must maintain the desired performance and safety characteristics at operating and transient conditions, and must be capable of accommodating transuranic elements for transmutation. Developing these fuels requires characterization, fabrication, and performance demonstration. Demonstration of actinide transmutation in a fast reactor requires fabrication of fuel containing actinides and irradiation of the fuel in a fast reactor to about 10% burnup. The demonstrations must show that the actinide-bearing fuel can be fabricated successfully via a remote process, performs reliably in the reactor, and has the necessary inherent safety characteristics. Because no fast reactor is operating today in the United States, the demonstration will require international collaboration. (Work performed primarily at Argonne-West currently supports the fabrication of samples of various actinide-bearing fuels for irradiation in both domestic and international facilities.)

*Advanced Reactor Technologies.* The central strategy of DOE's Generation IV program is to cooperate internationally to identify, assess, and develop (over the next three decades) nuclear energy technologies that can compete in many markets with the most cost-effective alternative technologies while improving nuclear safety, minimizing the impact of nuclear waste, and further reducing the risk of proliferation. The goal is one or more next-generation nuclear energy systems designed and deployable worldwide by 2030. Argonne — primarily at its Illinois site — contributes to the development of key

Generation IV technologies: the supercritical water reactor, the very-high-temperature gas-cooled reactor, the gas-cooled fast reactor, the lead-alloy-cooled fast reactor, and the sodium-cooled fast reactor. We will combine new technologies with our past experience in designing and operating fast reactors in order to contribute to designing Generation IV systems, including thermal- and fast-spectrum reactors. International collaborations will facilitate this work. Generation IV R&D aims to support a national decision on development of fast-reactor systems by 2010.

*Spent Fuel Treatment Facility.* The final component of this initiative is a facility designed, constructed, licensed, and operated to treat spent fuel from light-water reactors. The facility would be larger than that used to demonstrate separation technologies and annually would treat some 100–500 metric tons of heavy metal. The facility’s operation would further demonstrate the technical and economic viability of fuel recycling, particularly the fabrication of new fuel containing recycled actinides and the production of waste forms for disposal. In addition, the facility’s operation would reduce the amount of spent fuel destined for a geologic repository and would support the deployment of subsequent treatment facilities.

Primary support for Argonne’s Advanced Nuclear Energy Systems initiative will be sought from DOE-NE (AF). Required resources are summarized in Table III.5.

**Table III.5 Advanced Nuclear Energy Systems<sup>a</sup>**  
(\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
<b>Costs</b>							
Operating	32.0	26.0	18.0	18.0	18.0	19.0	19.0
Capital Equipment	8.0	5.0	4.0	3.0	3.0	3.0	3.0
Construction	-	-	-	-	-	-	-
Total	40.0	31.0	22.0	21.0	21.0	22.0	22.0
Direct Personnel	155.0	120.0	80.0	75.0	75.0	75.0	75.0

<sup>a</sup> FY04 includes funding from DOE’s Advanced Fuel Cycle Initiative and Generation IV program, for both Argonne-East and Argonne-West. FY05 includes a full year of funding at Argonne-East and four months at Argonne-West from both DOE programs. Projections for later years are for Argonne-East only.

## 2. Hydrogen Research and Development

In his 2003 State of the Union address, President Bush announced a major initiative to accelerate the development of a national hydrogen economy. The goal is to reverse America’s growing dependence on foreign oil by developing science and technology for commercially viable fuel cells that use hydrogen to power cars, trucks, homes, and businesses without directly emitting pollution or greenhouse gases. This national initiative encompasses basic scientific research and technology development for the widespread production, storage, and distribution of hydrogen and for its use in fuel cell vehicles, industrial production, heating, and electricity generation.

Achieving the President’s vision for our energy future requires an aggressive, interdisciplinary R&D effort that spans materials science, chemistry, and engineering. Before a hydrogen economy can become economically competitive, fundamental scientific breakthroughs are needed to dramatically improve the efficiency and effectiveness of hydrogen production, storage, distribution, and utilization. The President’s FY 2005 budget emphasizes the basic research required for this effort.

To support the national hydrogen initiative, Argonne has mounted a coordinated effort that integrates our state-of-the-art user facilities with our expertise in basic science, technology, and technology development and deployment. Central to our research program are two crosscutting objectives: (1) high-performance materials for hydrogen separation and fuel cell membranes and (2) new catalysts to improve hydrogen production and combustion. Our pursuit of these objectives draws on our broad knowledge of materials science and chemistry to coordinate research programs from basic to applied science. The unique capabilities of Argonne’s IPNS, APS, and Electron Microscopy Center are particularly valuable in our work on high-performance materials and catalysts.

To investigate hydrogen production from nuclear power, we will apply our extensive expertise in nuclear reactor technology. To address hydrogen utilization, we will take full advantage of experience and facilities developed

through our participation in the DOE-Energy Efficiency and Renewable Energy (DOE-EERE) FreedomCAR Partnership and DOE-EERE's program on stationary fuel cell systems for distributed generation by electric utilities. Our program builds on insights and research directions identified by two recent workshops: (1) the May 2003 DOE-BES Workshop on Hydrogen Production, Storage, and Use (report online at <http://www.sc.doe.gov/bes/hydrogen.pdf>), in which Argonne played a leading role, and (2) the August 2002 DOE-EERE Hydrogen Storage Workshop, which we hosted.

Argonne is already a leading DOE resource for developing technologies for hydrogen production, distribution, storage, and use. Relevant R&D programs supported by DOE and industrial collaborators include the following:

- Catalysts for hydrogen chemistry
- Economic and technical analysis
- Environmental research
- Fuel and power systems
- Fuel cell development and testing
- Hydrogen production
- Hydrogen storage
- Infrastructure assurance
- Technology validation projects
- Vehicle simulation and testing

Primary support for our Hydrogen Research and Development initiative will be sought from DOE-SC (KC); DOE-EERE (EE); DOE-Fossil Energy (AA); and DOE-NE (AF). Required resources are summarized in Table III.6.

**Table III.6 Hydrogen Research and Development**  
(\$ in millions BA, personnel in FTEs)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs							
Operating	10.0	12.0	14.0	16.0	24.0	24.0	24.0
Capital Equipment	-	0.5	1.5	3.0	3.0	2.0	1.5
Construction	-	0.2	2.0	2.0	2.0	1.0	1.0
Total	10.0	12.7	17.5	21.0	29.0	27.0	26.5
Direct Personnel	10.0	25.0	45.0	80.0	120.0	120.0	120.0

Our proposed Hydrogen Research and Development initiative has seven coordinated components: (1) catalysis for hydrogen chemistry, (2) hydrogen production, (3) hydrogen storage, (4) hydrogen utilization, (5) infrastructure development, (6) environmental research, and (7) technology validation.

*Catalysis for Hydrogen Chemistry.* Catalysis is ripe for fundamental advances through the use of modern experimental and theoretical tools that were unavailable even five years ago. The knowledge gained from these studies is expected to significantly improve the cost, performance, and reliability of many chemical processes needed for a hydrogen economy. Argonne will use a wide range of basic science tools, developed in our interdisciplinary research environment, to explore the atomic basis for catalysis of these chemical reactions. Our tools include (1) surface structure and excitation analysis using x-ray scattering at a novel *in situ* electrochemical cell at the APS, (2) nanoscale surface modification through lithography and self-assembly at the Center for Nanoscale Materials, (3) transmission electron microscopy at the Electron Microscopy Center, (4) local electronic structure analysis using scanning tunneling microscopy, and (5) quantum chemical theory and simulation for catalytic geometries.

*Hydrogen Production.* We will explore a variety of options for using domestic energy resources — fossil, nuclear, and renewable — to produce hydrogen efficiently. The main transition strategy to a hydrogen economy envisions the co-production of electricity and hydrogen from fossil fuels, with stringent environmental controls and carbon sequestration. To support this transition strategy, we will continue to develop fuel-processing technology as a near-term means of producing hydrogen from fossil fuels or from renewable fuels such as ethanol. Much of this fossil fuel research will also be applicable to the longer-term strategies for (1) co-generating electricity and hydrogen by nuclear power and (2) developing novel lower-temperature thermochemical cycles, high-temperature electrolysis, and advanced membranes that use heat from a nuclear power plant to generate hydrogen from water. By developing the next generation of nuclear reactors (Generation IV) in conjunction

with efficient hydrogen generation technology, we will address the nation's two major energy needs: electricity and transportation fuels. Argonne is the key contributor to DOE's development of an R&D plan for producing hydrogen from nuclear power.

*Hydrogen Storage.* A major challenge to the success of hydrogen-powered vehicles is the development of lightweight, compact, safe onboard hydrogen storage. Building on the DOE-sponsored Hydrogen Storage Workshop that Argonne hosted in 2002, we will explore new and innovative concepts for storing hydrogen. Laboratory-directed research is already investigating such novel concepts, and other ideas are being considered. Some of this research will benefit significantly from work at Argonne's emerging Center for Nanoscale Materials. We propose to lead a DOE-supported virtual center for hydrogen storage research through such novel approaches as chemical hydrides, metal-organic frameworks, and nanoclusters and nanofibers. We also propose to participate in other DOE virtual centers to investigate storage through use of carbon-based materials and advanced hydrides.

*Hydrogen Utilization.* Our work on hydrogen utilization will build on our extensive, wide-ranging partnerships with nonfederal organizations in areas crucial to developing this aspect of the hydrogen economy. We have conducted research with the automotive industry and its suppliers through the FreedomCAR Partnership, helped fuel cell companies develop products, worked with state and local government agencies on alternative-fuel demonstrations, and helped electric power companies analyze the

technological requirements for load management and transmission.

*Infrastructure Development.* In collaboration with Canadian partners in the "2050 Study," we are examining long-range supply-and-demand scenarios for transportation fuels. For our Hydrogen Research and Development initiative, we propose further technical and economic analyses focused on hydrogen distribution issues. Our expertise in infrastructure assurance enables us to identify the steps needed to ensure that a national network for hydrogen transmission and distribution is safe and secure.

*Environmental Research.* Environmental impacts from the transition to a hydrogen economy must be considered. We will draw on our broad expertise in environmental research to investigate largely unanswered questions regarding the possible atmospheric and global warming impacts of hydrogen leaks and other losses from vehicles and a national hydrogen infrastructure.

*Technology Validation.* DOE is soliciting partnerships to conduct cost-shared demonstrations of hydrogen-powered vehicles and of hydrogen production and other infrastructure. We will form a regional partnership with vehicle developers, energy suppliers, and vehicle fleet operators for needed hydrogen technology demonstrations. In addition, Argonne and the Idaho National Engineering and Environmental Laboratory will collaborate to build and operate a hydrogen technology testing facility and, eventually, a demonstration facility to produce hydrogen by using heat from nuclear power.



# IV. Science and Technology Strategic Plan

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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.

The chapter is organized in terms of strategic plans for each of 20 planning units that span our major mission areas (see the inset box). These R&D area strategic plans are grouped into fundamental science and national research facilities, energy and environmental technologies, and national security. This grouping encompasses DOE's four mission areas. In addition, the chapter concludes with crosscutting discussions of collaborative R&D partnerships and the Laboratory Directed R&D Program.

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.

## A. 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.

## 1. 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

### Argonne's Strategic Plans

#### A. Fundamental Science and National Research Facilities

1. Advanced Photon Source
2. Materials Science
3. Chemical Sciences
4. Nuclear Physics and the Argonne Tandem-Linac Accelerator System
5. High-Energy Physics
6. Mathematics, Computing, and Information Sciences
7. Intense Pulsed Neutron Source
8. Biosciences
9. Environmental Research
10. Science and Engineering Education and University Programs

#### B. Energy and Environmental Technologies

1. Advanced Nuclear Technology
2. Energy and Industrial Technologies
3. Transportation Technologies
4. Environmental Treatment Technologies
5. Energy and Environmental Systems
6. Biotechnology

#### C. National Security

1. Nuclear National Security
2. Homeland Security
3. National Defense

#### D. Collaborative R&D Partnerships

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 2003 over 2,700 unique users performed work there. International competition in this research area 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 than a quarter billion dollars in capital investments for construction of APS beamlines.

As of the summer of 2004, 30 of 34 available sectors were assigned to partner users. (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: 1 by the Structural Biology Center Collaborative Access Team and the remaining 6 by the X-ray Operations and Research section of the APS. The latter 6 sectors have been developed and instrumented for research in materials science, chemical science, atomic physics, and condensed matter physics. Techniques employed include small-angle scattering, high-energy x-ray scattering, x-ray microbeam, nuclear resonant scattering, high-resolution inelastic scattering, coherent imaging, and magnetic scattering using polarized x-rays. In addition to the 7 sectors discussed above, the APS currently shares responsibility for operating 3 other sectors. This number is expected to grow.

The APS is involved in the construction of several new beamlines, including the Nanoprobe beamline associated with the Center for Nanoscale Materials (CNM); an inelastic scattering beamline

(sector 30); and a dedicated, high-resolution powder diffractometer on the bending magnet of sector 11. The expectation is that the APS will be responsible for operating these three beamlines.

Demand for the four unassigned sectors at the APS is high. Decisions regarding their assignments will be made over the next several years. A retreat being organized for the summer of 2004 will bring together current and potential users to discuss options.

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 2003 the availability of APS beam time (the percentage of scheduled user beam time actually delivered) was nearly 98%.

### *Vision*

The APS will continue to operate at current high reliability levels and will remain the preminent 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 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 beamline.

Until FY 2004, all sectors assigned to partner users at the APS had an associated laboratory-office module (LOM) to house operational staff

and provide laboratory space for sample preparation. In FY 2003, the Nanoprobe beamline and the inelastic scattering beamline were each assigned an additional sector. The CNM being constructed adjacent to the APS Experiment Hall will provide the support laboratories and office space for the staff and users of the Nanoprobe beamline. However, there is currently no LOM to support the inelastic scattering beamline and the remaining unassigned sectors. Funding for the final LOM 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 unassigned 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	7.8	8.0
Capital	11.4	14.4	22.0	21.8	21.0	20.0	24.7	29.5
Equipment								
Construction	-	-	-	-	-	-	-	-
Total	15.0	20.0	30.0	30.0	30.0	27.5	32.5	37.5
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 have developed 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)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
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	-	-	-

**2. Materials Science**

*Situation*

Our research in materials science draws from diverse intellectual resources in the Materials Science, Chemistry, and Bioscience Divisions; from highly developed capabilities in synthesis, experiment, theory, and simulation; and from the rich variety of sophisticated instrumentation at Argonne’s user facilities — the Electron

Microscopy Center (EMC), the Intense Pulsed Neutron Source (IPNS), the APS, and the CNM. This broad base of resources and capabilities provides a stimulating and fertile environment for pursuing new directions in the design, preparation, characterization, and understanding of materials.

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

The impact and prestige of our scientific program was highlighted in 2003 by the awarding of the Nobel Prize in Physics to Alexei Abrikosov. In addition, Argonne scientists received two prestigious international prizes — the John Bardeen and Kamerlingh Onnes Prizes — and three national awards for scientific and technical accomplishment.

*Vision*

Materials research at Argonne will foster world-class science, forefront instrumentation, and unique user facilities that support the DOE mission. We will pursue our research through coordinated scientific teams that integrate materials synthesis, sophisticated experiment, conceptual theory, and numerical simulation. Our contributions to new materials, especially at the nanoscale, will provide vital support to 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 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 an aberration-corrected transmission electron microscope (TEM) 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. More particularly, we continuously refresh our program mix by adding new directions as new materials are discovered and research capabilities grow. We also stress comprehensive programs that incorporate integrated experimental and theoretical thrusts and exploit advanced scientific instrumentation ranging from benchtop scanning probes to unique instrumentation at electron, x-ray, and neutron sources. In addition, 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 both intellectual stimulation and 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 IPNS, the new CNM (see Section III.A.1), and Argonne's advanced computing research facilities. 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 for peer review. 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 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 installing 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 developing 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 it 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 our 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 state-of-the-art laboratories designed to have quiet floors, electromagnetically shielded rooms, and precise temperature control. Ideally, a new, dedicated,

noise-free building would be located near complementary facilities such as the CNM. Experimental samples fabricated in the CNM could then be characterized conveniently by using the electron microscopy.

***Initiative: Transmission Electron Aberration-Corrected Microscope***

Thanks to advances in aberration correction and quantitative-transmission electron microscopy, a new generation of electron microscopes can be built that (1) are capable of sub-angstrom image resolution and sub-electron-volt spectroscopic resolution and (2) 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, together with the microscopy group at Brookhaven National Laboratory. Each group will contribute 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 microcharacterization 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 succeeding workshops in FY 2002 and FY 2003, 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.

### **3. Chemical Sciences**

#### *Situation*

Chemistry is an Argonne core capability closely interrelated with research in materials science, bioscience, computer science, and the emerging field of nanoscience. World-class research programs employ staff with cutting-edge expertise to study fundamental scientific questions critical to DOE's mission. This research provides essential foundations for addressing issues of energy independence, environmental sustainability, and national security, especially by enabling new technologies for energy efficiency, energy conversion, combustion, nanotechnology, catalysis, and cleanup and disposal of radioactive and nonradioactive wastes.

#### *Vision*

We will enhance our chemical science research by strengthening our leadership in established research focus areas, by developing new initiatives, and by forging new collaborations within Argonne and with major university research centers, especially the University of Chicago. We will emphasize multidisciplinary, multiscale chemical research of broad reach.

*Objectives*

Our central goal is to foster cross-disciplinary collaborations that will implement revolutionary approaches to difficult problems in chemical science. Major long-range objectives of our core research program are as follows:

- Through studies combining experimentation and theory, improve understanding of the chemical reactivity and physical properties of nanoscale materials, including gas-phase clusters, inverse micelles, colloids in solution, hybrid bioinorganic systems, and nanomaterials on or in bulk phases. Achieving this objective is greatly facilitated by collaboration with Argonne's CNM, by participation in the Consortium for Nanoscale Research with the University of Chicago, and by a catalysis research collaboration with Northwestern University that includes joint appointments.
- By combining experimentation with theory and computation, deepen understanding of chemical reactivity at the molecular level in both the gas and condensed phases and at the interface between phases.
- Improve understanding of the fundamental physicochemical phenomena that occur when radiation interacts with matter, in the context of
  - Photochemical energy conversion in natural and biomimetic photosynthetic systems;
  - Charge dynamics and transport in condensed phases;
  - Studies of gas-phase photoionization and photodissociation; and
  - X-ray interactions with atoms, molecules, and complexes.
- Develop understanding of the chemical reactivity, physical properties, and separation chemistry of species containing f-electron atoms, especially the actinides.

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

- Specialized capabilities at the APS in areas including transient x-ray scattering and spectroscopies; hard x-ray physics in intense laser fields (atomic, molecular, and optical); and experiments involving samples containing actinide elements, conducted at our Actinide Facility
- Novel electron and x-ray generators capable of subpicosecond time resolution
- Facilities for transient optical spectroscopies and time domain, multifrequency investigations of electron paramagnetic resonance
- 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 science research programs integrate special expertise with unique tools and facilities. The recent developments described below are establishing new research directions that serve DOE's energy mission:

- We are investigating new ideas about hydrogen production, storage, and use, building on our recent discoveries in such diverse areas as the synthesis of template-derived carbon nanofibers, the reducing power of irradiated metal oxide colloids, and biochemical processes for hydrogen removal. (See the major Laboratory initiative Hydrogen Research and Development in Section III.B.2.)
- Our developing capabilities for synthesizing nanoparticles allow us to address fundamental questions about reactivity and promise novel approaches to organized assembly. We are also developing and applying tools to study electronic structures in confined spaces, to observe the migration of charge and spin, to characterize and control photonics by the synthesis and arrangement of metal nanoparticles, and to understand the high efficiency and selectivity of catalysis on the molecular scale.

- We are gaining valuable experience in research areas at the inorganic-biochemical interface; in state-of-the-art time-resolved x-ray capabilities on molecular and kinetic time scales; in construction and application of the tabletop terawatt laser for ultrafast pulse radiolysis; and in computational chemistry — by using the rapidly expanding power of local and remote parallel computing facilities. The resulting synergistic capabilities provide a critical mass for addressing issues in complexity and in collective phenomena, including (1) particle aggregation and disaggregation in inorganic systems and (2) protein dynamics in biological systems.

In addition to DOE-BES, we will explore a broad range of further sponsors for studies in these new directions.

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

In collaboration with several universities, we have developed a new program in computational nanophotonics that is supported by a competitive

award from DOE's Computational Nanoscience program. The program will focus on developing and applying software for problems in nanophotonics and nanoelectronics. The software will apply mainly to continuum models but also to atomistic models. It will be tested on realistic applications and later distributed widely.

Our integrated program in the fundamental chemistry of radioactive waste is partly supported by the DOE Environmental Molecular Sciences Institute, through which we collaborate with the University of Notre Dame. This program exploits our unique core capabilities in chemical separations science, heavy-element chemistry, radiation chemistry, and theoretical chemistry, as well as our facilities for research with radioactive materials, including the Actinide Facility at the APS and a special nuclear magnetic resonance facility. This is the largest of a growing number of university-led actinide research collaborations that involve many students in actinide research.

We partner with Northwestern University in the Institute for Environmental Catalysis. The institute's leader, Professor Peter Stair, now has a joint appointment with Argonne. This partnership takes advantage of our facilities at the APS for magnetic resonance, pulse radiolysis, and synchrotron research and our expertise, especially in synthesis using cluster deposition and atomic layer deposition. The partnership also exploits the two institutions' experience in both heterogeneous and homogenous catalysis, and it will increasingly take advantage of the emerging capabilities of the CNM.

We have developed two programs in computational chemistry in response to DOE's Scientific Discovery through Advanced Computing initiative. The first involves participation in the Collaboratory for Multiscale Chemical Sciences, a collaboration with Sandia National Laboratories and several universities. This program will develop software for providing internally consistent "active" tables of thermodynamic values. (Unlike existing tables, active tables allow users to test the implications of thermodynamic values.) The second 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.

#### 4. 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 (RIA), 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) studies of relativistic heavy-ion collision dynamics using beams from Brookhaven's newly commissioned RHIC (Relativistic Heavy Ion Collider); (4) nuclear theory, which focuses on developing fundamental understanding of hadronic and nuclear structure, reactions, and dynamics; and (5) accelerator R&D, especially on applying superconductivity radio frequency techniques to ions and on producing and accelerating radioactive beams.

##### *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 the national RIA facility, which will be based largely on novel superconducting accelerator technology originally developed at the Laboratory and used for ATLAS. Our accelerator physicists are conducting a broad range of R&D to establish the technological basis for the RIA facility. (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 IBM SP at the National Energy Research Scientific Computing Center, 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, RHIC, and the planned RIA facility.

### *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. 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. An accelerator improvement project now under way will increase the facility's beam energy by about 25%.

#### *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 are 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.) By capitalizing on R&D for RIA, we are planning a near-term initiative to add another unique capability to the ATLAS facility. The basic idea is to capture and reaccelerate ions resulting from the spontaneous fission of californium.

## **5. 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. Argonne plans to continue operational support and physics analysis until the end of data taking in mid 2007. An Argonne physicist currently serves as spokesman for the collaboration.

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 (NSF). Some work on the ATLAS detector has shifted to preinstallation and installation activities that should be completed in 2006. 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. MINOS employs a neutrino beam from the new Fermilab main injector, and it 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 are 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 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 installation of the detector at the CERN Laboratory. We are also currently contributing to the design and prototyping of the trigger for the ATLAS detector. 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-NSF 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 capabilities.

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)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs							
Operating	0.8	1.0	1.5	2.0	2.5	3.0	3.0
Capital Equipment	0.3	0.3	1.0	1.3	1.5	2.0	2.0
Construction	-	-	-	-	-	-	-
Total	1.1	1.3	2.5	3.3	4.0	5.0	5.0
Direct Personnel	4.0	5.0	8.0	11.0	13.0	15.0	15.0

## 6. Mathematics, Computing, and Information Sciences

### *Situation*

The nation has reached a critical junction in its ongoing quest for scientific excellence and leadership. The scientific and engineering communities have embraced computational simulation as an essential tool for scientific progress. Solutions to hundreds of important but currently intractable problems are almost within our grasp, including reliable predictions of climate change at the regional scale, comprehension of plasma turbulence, molecular modeling of cell mechanisms, simulation of large molecules encountered in nanoscience, and accurate simulation of supernova explosions. However, solutions to all of these problems require more computing capability than currently exists, by an order of magnitude. Moreover, reports from the scientific computing community<sup>1</sup> document a need for sustained computing performance of more than 50 teraflops in 2006 and approaching one petaflop ( $10^{15}$  operations per second) by the end of the decade, in order for the United States to maintain its leadership position in many areas of computational science and engineering.

A satisfactory path to petascale computing is not a simple matter of waiting for the technology to arrive from the normal progress of commercial R&D. The entire U.S. computing research

<sup>1</sup> See the following key reports:

- *Revitalization of High-End Computing* (National Coordination Office for Information Technology Research and Development, April 30, 2004, linked at <http://www.itrd.gov/>).
- *A Science-Based Case for Large-Scale Simulation* (DOE Office of Science), Volume 1 (July 30, 2003, linked at <http://www.pnl.gov/scales/>), Volume 2 (to be published).
- *Scientific Discovery through Advanced Computing* (DOE Office of Science, March 24, 2000, linked at <http://www.osti.gov/scidac/mission.html>).
- *The Challenge and Promise of Scientific Computing* (DOE Office of Science, December 2003, online at [http://www.science.doe.gov/Sub/Occasional\\_Papers/1-Occ-Scientific-Computation.PDF](http://www.science.doe.gov/Sub/Occasional_Papers/1-Occ-Scientific-Computation.PDF)).

community has many challenges to overcome, including the following:

- *Scalability.* As we approach the limits of speed-of-light communication and power delivery systems, future systems will have between 10,000 and 100,000 individual processors, implying more complexity, by at least an order of magnitude, than current systems and software can demonstrably manage and effectively use.
- *Technological Limitations.* Current technologies, such as clusters and parallel vector processing, appear to be incapable of scaling effectively to the petaflops regime. Innovative architectures, such as virtual-vector and system-on-a-chip technologies, therefore must be explored.
- *Economics of Computer Architectures.* A decade ago, U.S. companies were producing supercomputers finely tuned for scientific and technical applications. In recent years, however, scientific computing has become increasingly dependent on — and limited by — hardware that is designed and optimized for commercial applications.

We believe that advances in computer science and applied mathematics are fundamental to solving these problems and delivering the computing capability the nation needs.

#### *Vision and Goals*

Our goal is to open a sustainable path to effective computing at the petaflops level and beyond. At the same time, we believe that, for certain classes of problems, distributed (Grid) computing is a compellingly efficient alternative to single-system petascale computing and that distributed computing can support science in other innovative ways.

#### *Objectives*

Achieving our vision will require the development of world-class supercomputing and networking resources, complemented by world-class algorithms, tools, and software. Argonne has established the following specific objectives for achieving a world-class computing capability:

- Work with DOE to formulate a national strategy for creating new computer designs that maximize 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, particularly by exploring design tradeoffs and testing early prototypes.
- Address key challenges in 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 advanced architectures.

#### *Issues and Strategies*

Argonne computing science researchers are at the forefront of U.S. scientific computing. Recently, we established a collaboration with Oak Ridge National Laboratory to develop a DOE-funded national-scale leadership computing facility, designed to enable a new scientific simulation capability for the country. Our particular interest is the IBM BlueGene architecture, which has the potential to scale far beyond current systems and to enable researchers to attack key scientific problems in diverse disciplines. The first BlueGene systems will ship in late 2004, and current plans call for one to be delivered to Argonne as an early testing platform. If this line of systems is successful, it has the potential to scale to one petaflop in a 100,000-processor system by 2008.

Distributed, or Grid, computing will be as important as faster computers in solving major scientific problems in the coming years. Distributed computing links workstations and parallel computers, large databases, and virtual-reality devices worldwide. Our deployment of the Globus Toolkit<sup>®</sup> has made Argonne the

international center of research on distributed systems. We are now exploring ways of extending this technology to areas of computational science such as a BioGrid. We are also taking the lead role in developing Grid technology for many projects funded by the federal program Scientific Discovery through Advanced Computing (SciDAC), including the Earth System 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 are the development and deployment of a petascale experimental research facility targeted at solving 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 initial primary applications areas for the petascale facility are the biosciences and nanosciences.

Argonne also has established the Laboratory Computing Project to promote the widespread use of high-performance computing technologies in many areas of science and technology across the Laboratory. As part of this project, Argonne has funded installation of a teraflop-class computing cluster. The system, called "Jazz," was chosen because it is highly reliable and easily reconfigured, two features essential for heavy production computing use. More than 50 projects are using Jazz to attack challenging computational science problems ranging from bioscience and climate modeling to nanoscience and nuclear engineering.

## 7. 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 2002 and FY 2003, 230–250 scientists conducted a total of approximately 400 experiments at the facility. In FY 2002 a total of 680 scientists participated in the experiments conducted.

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 26 weeks in FY 2003, and it is scheduled to operate for 25 weeks in FY 2004.

### *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 research on condensed matter 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 CNM, the IPNS will further increase its scientific productivity.

### *Issues and Strategies*

The IPNS has historically been over-subscribed, understaffed, and underfunded. The additional \$4 million in IPNS operating funds included in DOE's Scientific Facilities Initiative beginning in FY 1996 now allows 25–27 weeks of operation per year, with a full complement of instruments serving users. Significant improvements in capital funding have enabled us to embark on a program of enhancing our instrumentation so we can continue to provide world-class capabilities.

Currently, two DOE facilities and a facility at the National Institute of Standards and Technology (NIST) provide neutrons to the user community: the IPNS, the Los Alamos Neutron Science Center 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, also at Oak Ridge, is scheduled for completion in FY 2006, with full user access scheduled for FY 2008.

Investments in instrumentation and facilities will allow the IPNS to continue providing world-class neutron data for the scientific community by further leveraging the facility's unique strengths. These strengths include the following:

- Very cold neutron spectra from liquid and solid methane moderators
- Wide wavelength bandwidth
- Polarization devices
- Low neutron background
- Co-location with the APS and CNM

We are undertaking an instrument enhancement project for the IPNS. As a whole, current and planned enhancements will greatly increase the facility's scientific capabilities. The resulting increased data rates, along with the development of capabilities unavailable elsewhere in the United States, will significantly broaden the range of scientific investigations that can be undertaken. Our development plan addresses all aspects of the IPNS facility where cost-effective improvements can yield tangible gains in the short term. These gains will be both in scientific throughput ("more science") and in scientific capabilities ("new science").

The enhancement plan anticipates, or has already achieved, the typical gains in data rates summarized in Table IV.4.

These improvements to the IPNS will enable important new types of scientific measurements and studies:

- Measurements of neutron scattering patterns  $S(Q, E)$  as a function of length scale ( $Q$ ) and energy ( $E$ ) on single crystals, glasses, and liquids

**Table IV.4 Typical Gains in Data Rates Anticipated or Achieved with IPNS Enhancement Plan**

Instrument	Data Rate Gain Factor	Status
<b>Current Instruments</b>		
Glass, liquids, and amorphous materials diffractometer (GLAD)	× 2	Planned
General-purpose powder diffractometer (GPPD)	× 15	Completed
High-resolution medium-energy chopper spectrometer (HRMECS)	× 4	In progress
Quasi-elastic neutron spectrometer (QENS)	× 32	Completed
Small-angle neutron diffractometer (SAND)	× 6	Completed
Single-crystal diffractometer (SCD)	× 16	In progress
Special-environment powder diffractometer (SEPD)	× 9	Planned
<b>New Instruments</b>		
Small-angle diffractometer (SAD) to small-angle spectroscopy instrument (SASI)	× 4	In progress
Nuclear beamline Test station		Planned
MiDaS (diffractometer with polarizer)		Planned

- Simultaneous structural and spectroscopic measurements over a wide  $Q$  range (i.e., over a length scale of  $0.4\text{--}2.5 \text{ \AA}^{-1}$ )
- Polarized-neutron SANS (small-angle neutron scattering) studies of magnetic nanostructures
- SANS studies on polymer and magnetic thin films
- Powder diffraction studies of complex materials such as pharmaceuticals
- Fast parametric studies on powders (in minutes)
- Studies of the dynamics of low-dimensional magnetic systems
- Diffuse-scattering studies
- Studies of magnetic structures and large cells
- More detailed probing in magnetic layers and interfaces

## 8. Biosciences

### *Situation*

Argonne is becoming a leader in methods for characterizing the structure and function of biological molecules. However, to achieve world prominence in 21st century biology, the Laboratory must augment its existing expertise and facilities and use those capabilities for groundbreaking studies of biomolecular systems' functions. This biosciences research will increasingly depend on interdisciplinary interactions with scientists in the fields of computation, physics, chemistry, and materials science. It will also depend on implementing high-throughput techniques for characterizing biomolecular systems to overcome experimental challenges that are currently unapproachable. Moreover, integrating the resulting data into a complete view of cellular behavior will require novel approaches to simulating complex systems. The required fusion of functional genomics with high-end computational simulation of molecular behavior in biomolecular systems is now widely called systems biology.

Five existing or developing programs and facilities at Argonne contribute importantly to our efforts in the biosciences:

- Our *Functional Genomics Initiative* (Section III.A.3) is currently enabling the development and use of novel strategies for characterizing macromolecular functions. This research includes significant efforts in structural and functional genomics, membrane protein expression and crystallography, affinity reagent generation, combinatorial biology, mapping of protein-protein and protein-small molecule interactions, nanobiotechnology, and other genome-wide approaches to biological problems.
- The *APS* provides unique capabilities for analyzing macromolecular structure and function through crystallography, solution scattering, and x-ray spectroscopy and imaging. The Structural Biology Center at the APS is the world's premier facility for crystallographic analysis of macromolecular

structures. The APS sector GM/CA CAT, currently under construction, will add three beamlines for protein crystallography.

- The *Midwest Center for Structural Genomics* is the most productive of the centers for structural genomics funded by the National Institutes of Health (NIH). Its investigations of proteins exploit high-throughput cloning, expression, purification, crystallization, and structure determination. High-throughput techniques pioneered in the center serve as prototypes for the extensive automated methods that will become increasingly crucial for biological research.
- The *Great Lakes Research Center of Excellence in Biodefense*, a program of the University of Chicago recently funded by the NIH and the state of Illinois, includes significant Argonne work. This program will play a central role in activities at the Regional Biocontainment Laboratory — the Ricketts Center, a University of Chicago facility funded by the NIH — to be sited at Argonne.
- Biology increasingly depends on computational resources for the management, analysis, and interpretation of data. Information technology is becoming sufficiently powerful to deal with the full complexity of biological systems. The facilities and expertise in Argonne's *Mathematics and Computer Science Division* will make critical contributions to all aspects of our future biology programs.

### *Vision*

Over the next two decades, Argonne will become one of the world's leading centers for the genome-wide analysis of biomolecular function by making ground-breaking contributions to understanding the molecular basis of cellular activities. To achieve this vision, we will use our extensive expertise in biology, chemistry, materials science, mathematics, and computer science — as well as our world-class experimental and computational facilities — in a coordinated, multidisciplinary effort to answer fundamental questions about the actions of biomolecular systems.

*Objectives*

To become a premier center for the functional characterization of biomolecular systems, we will build on our current work in structural and functional genomics; our planned efforts in protein production and characterization; our interactions with the Great Lakes Research Center of Excellence in Biodefense and the Regional Biocontainment Laboratory; and our enhanced involvement of materials scientists, computer scientists, and — in the area of molecular design and engineering — Argonne's emerging CNM. New facilities will be required to house the integrated research teams implementing these interactions; several are currently being planned.

Central to our program is the planned Protein Production and Characterization Facility. This high-throughput facility for producing proteins and affinity reagents and for comprehensive, genome-wide characterization of protein function (see Section III.A.3) will enable complex experimental approaches to studying macromolecules, macromolecular assemblies, and cellular subsystems. The facility will produce reagents that make possible a broad range of studies on the molecular basis of cell function and will enable exhaustive studies of molecular function that are currently impossible.

Our work in structural genomics, primarily located at the Midwest Center for Structural Genomics, is expected to grow significantly in coming years. To accommodate this growth, we have proposed that the state of Illinois fund an Advanced Protein Crystallization Facility where very-high-throughput crystallization and crystallographic analysis of proteins will be performed.

Accelerated protein production will inevitably increase demands for protein characterization facilities. For that purpose, one of the remaining APS sectors should be developed to exploit the extraordinary power of x-ray scattering, spectroscopy, and imaging. This GTL CAT would combine an undulator beamline for wide-angle x-ray scattering and x-ray spectroscopy (XAFS) and a second undulator beamline for x-ray imaging (in particular, for x-ray fluorescence imaging at resolutions comparable to those of the nanoprobe beamline of the CNM). A bending magnet beamline would be used for small-angle

scattering and fiber diffraction from partially ordered, partially oriented materials.

*Issues and Strategies*

Key to understanding cellular action is understanding the functioning of proteins — the molecules that carry out virtually all the cell's activities — and understanding the integration of those functions in support of cellular action. Sequencing the DNA of genomes has revealed the full inventory of proteins encoded by many species and has provided a global framework for the functional analysis of organisms at the molecular level. However, though sequencing provides clues about the functions of many proteins, sequencing alone cannot support a complete understanding of cell function.

Cellular actions are manifestations of a series of coordinated molecular steps, each involving the functioning of dozens, or even hundreds, of proteins. Biology in the 21st century is fundamentally about understanding the molecular basis of these actions, which will require both comprehensive understanding of the functions of individual molecular components and detailed characterization of their interactions. Over the next 20 years, biology will focus on integrating understanding of molecular function into understanding of progressively larger, more complex cellular subsystems. Biological research increasingly will rely on high-throughput experimental methods and advanced imaging systems to collect vast amounts of data; it will also rely on new computational approaches to organizing and integrating those data and to constructing detailed models of system-level function. Progress will depend on interdisciplinary research teams, large-scale robotic instrumentation, and high-end computation.

The future of biological sciences will depend critically on close cooperation among the biological, physical, and computational sciences, taking full advantage of the increasingly complex tools of these fields. At Argonne, biological research will take advantage of (1) unique tools that include the APS, the IPNS, and high-end computing resources; (2) opportunities for interaction with the Laboratory's superb programs in nanoscience, chemistry, physics, and

computational science; and (3) a management structure that fosters application of large-scale science to address problems where study by isolated individual investigators would be impracticable or inefficient.

Beyond studies aimed at a better understanding of biological systems, we see a tremendous opportunity to apply our understanding of biomolecular systems to designing and fabricating complex nanostructures. This effort will involve all of the physical and biological sciences that investigate the properties of materials at the nanoscale, in order to elucidate the behavior of complex molecular systems and to develop the principles of molecular design and engineering needed to fabricate the next generation of nanoscale devices.

## 9. 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, our 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 of aerosol formation, transformation, and transport as they relate 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 below-ground 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 NSF (through collaborations with university partners), and the Department of Defense.

Required resources are summarized in Table IV.5. 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.5 Challenges in Environmental Science**  
(\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
<b>Costs</b>							
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
<b>Direct Personnel</b>	3.0	5.0	9.0	14.0	20.0	25.0	25.0

**10. 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. At the university level, core programs provide opportunities for research participation by outstanding undergraduates and faculty, summer schools for

graduate students at designated user facilities or in cutting-edge technology development programs of interest to DOE, and opportunities for thesis research by graduate students. 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 representing the “best of the best” 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). Recently, our role expanded to include placement of IAEA fellows in R&D programs throughout the country. As in earlier years, we develop and conduct courses in peaceful applications of nuclear technology. We also provide technical support to the Department of State and the IAEA.

#### *Vision*

We will enrich science education and workforce development 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 workforce development are as follows:

- Continue to attract to our research participation programs a large, diverse pool of highly qualified undergraduate students who are among the “best of the best.”
- 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, postdoctoral fellows, and faculty into Laboratory research programs and emerging DOE initiatives through internships and training activities.
- Provide training and fellowship 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 workshops 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 infrastructure 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 students and teachers is being 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.

## B. 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.

### 1. 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 Energy Systems. 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) DOE’s Advanced Fuel Cycle Initiative, which aims to close the nuclear fuel cycle with new technology that is environmentally sound, proliferation resistant, and economical; (2) DOE’s Generation IV R&D program, whose objective is a new generation of nuclear reactors for deployment before 2030; and (3) the International Nuclear Safety Program, 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. The Nuclear Energy Research Initiative (NERI), one of the main nuclear R&D programs in recent years, is being integrated by DOE into its Advanced Fuel Cycle Initiative and its 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.

#### *Issues and Strategies*

Argonne-West is to be transferred to the new Idaho National Laboratory in January 2005. Nevertheless, plans call for continued close integration of the research on advanced nuclear technology conducted in Idaho and Illinois.

Key strategies for our nuclear technology programs include the following:

- Undertake the major Laboratory initiative Advanced Nuclear Energy Systems, 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 of the National Aeronautics and Space Administration in fission reactors for space missions.
- Continue to participate in key programs of the DOE Office of Nuclear Energy, Science and Technology (DOE-NE): nuclear technology, Nuclear Energy Plant Optimization, the Advanced Fuel Cycle Initiative, Generation IV R&D, and the Nuclear Hydrogen Initiative. Also participate in international collaborations under these programs. Apply Argonne's nuclear expertise and unique facilities to current, near-term, and longer-term future nuclear technologies; apply our expertise to critical issues affecting the continued safe and efficient operation of existing nuclear power plants.
- Within our areas of special expertise, participate in advanced technology R&D programs such as DOE's 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 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.

In addition to the future work discussed above, Argonne proposes the initiative International Nuclear Safety Program.

***Initiative: International Nuclear Safety Program***

We support the International Nuclear Safety 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 Soviet-designed power reactors, and the lessons learned are applicable to many other nuclear facilities around the world. Therefore, we propose to expand our current program to collaborate with countries wishing to 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 will include collaborative training, coordinated between Argonne and the IAEA, that facilitates the transfer of safety assessment technology to participating countries. The program will also link participating countries through collaborative research.

Resource requirements are given in Table IV.6. Funding from DOE-NE (AF-15-30) would be supplemented by funding from the U.S. Agency for International Development.

**Table IV.6 International Nuclear Safety Program**  
(\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
<b>Costs</b>							
Operating	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
<b>Total</b>	<b>1.0</b>						
<b>Direct Personnel</b>	<b>3.0</b>						

**2. 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.B.3), “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.

*Industrial Technologies Program.* 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 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 nanocrystalline 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, and support companies implementing that software; 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<sub>2</sub>O<sub>3</sub>, and CeO<sub>2</sub> — 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 Industrial Technologies Program, 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
- Aluminum: Aluminum Association; the company SECAT LLC
- Metal casting: Cast Metal Coalition
- Glass: Glass Manufacturing 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.B.6.

*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 2005 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 2005 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.

### 3. Transportation Technologies

#### *Situation*

The world's transportation system depends critically on petroleum. Oil supplies 96% of the energy used to move people and goods, and demand has risen 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 China, India, and other developing economies grow. In less than 20 years, China's consumption of oil will be second only to that of the United States. The price of transportation fuels is expected to rise faster than general inflation, making vehicles with greater energy efficiency increasingly important.

Two major research programs led by DOE are designed to reduce oil demand by developing vehicles with greater energy efficiency: the FreedomCAR program and the Hydrogen 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](http://www.transportation.anl.gov)).

#### *Vision*

Transportation and energy infrastructure will always be critical to U.S. national security. Argonne's Transportation Technology R&D Center will become the premier 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 through basic research, technology development, and 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 Hydrogen Fuel Initiative (spearheaded by the DOE Office of Energy Efficiency and Renewable Energy, in partnership with Ford, General Motors, and DaimlerChrysler) to
  - Improve the energy and emissions of conventional vehicles through better combustion, alternative fuels or new fuel blends, and advanced materials;
  - Ensure reliable systems for future fuel cell powertrains, with costs comparable to those of conventional engine and powertrain systems; 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 various fuels and engines.
- Develop new technology with a private-sector partner — General Motors Electromotive 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, which is both 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, which are their 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 the performance and emissions of actual vehicle systems.
- *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. We are also developing solid oxide fuel cells for transportation use. Our Fuel Cell Test Facility is capable of testing fuel cells up to 50 kW in size.
- *Energy Storage Devices.* In response to stringent environmental regulations, we are developing advanced batteries for hybrid 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 at the APS by using the world's brightest x-rays promise improved understanding of combustion and soot formation, leading to the development of cleaner and more efficient engines.
- *High-Performance Computing.* Argonne has supported the transportation industry with state-of-the-art computational capabilities in fluid mechanics, solid mechanics, dynamic simulations, and multidisciplinary design optimization. Major analyses are considering underhood cooling, aerodynamics, engine combustion, 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. In general, use of the APS is expected to be very valuable in the development of catalysts and other new transportation materials.

#### 4. 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).

##### a. 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 application to the complete inventory of EBR-II sodium-bonded fuel; that work is 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. In FY 2003 that work was incorporated into DOE's Advanced Fuel Cycle Initiative and broadened to include demonstration of pyroprocessing and technology for application beyond the processing of EBR-II spent fuel. Processing rates for EBR-II spent fuel have been 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 will be increased. The capacity rate of 5 metric tons per year may be reached after processing improvements are implemented and staffing is increased. In February 2005 these activities will become part of the Idaho National Laboratory.

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 short-term tests, as well as 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.

## **b. 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, the 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 continue to perform solid core sampling of contact-handled transuranic materials (homogeneous solids or soils and gravels). Begun in 2003, this work is being performed in the Waste Characterization Area of the Hot Fuel Examination Facility (HFEF). In the DOE complex, about 700 waste drums are estimated to require core sampling. This work is scheduled to be completed before the end of the decade.

We propose construction of 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 the Idaho National Engineering and Environmental Laboratory (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 project will augment the capabilities of Argonne-West in important ways. The project will include an addition to the HFEF, and current support capabilities at the HFEF — such as cask handling — will be integrated into the RTF.

The mission need for the RTF has been confirmed by DOE-NE, and Argonne's proposal is being considered as one of several options for meeting that need at INEEL. Inclusion of funding for RTF design and construction is expected in DOE's FY 2006 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.

### c. 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, Korea, 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, other government organizations, 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.

## **5. 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 and to integrate diverse resources. We address complex 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 relevant engineering specialties and the physical, biological, and social sciences.

Energy and environmental problems create these challenging national needs:

- The complexity of energy systems, in conjunction with related environmental issues such as water resources, necessitates a multidisciplinary, integrated approach.
- 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 discern, merge, and display only the more 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 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; through effective communication of options to policy makers; 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:

- Develop models, methodologies, and techniques that give decision makers relevant and accurate information about the changing structure of the energy system.
- Provide tools to support federal managers, policy makers, and private-sector businesses facing new regulatory requirements, especially by integrating environmental assessments, risk analyses, and cost-benefit analyses.
- 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, apply 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*

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

- Investigate the application of advanced techniques — such as complex adaptive systems analysis and agent-based simulation — to providing better decision making information in the rapidly changing, highly complex, nonlinear arena of energy and environmental policy.
- Create cost-effective approaches to site cleanup and long-term stewardship by synthesizing better site sampling strategies, better monitoring methodologies, and more flexible decision-making practices based on rapid acquisition, synthesis, and evaluation of accurate field data.
- Anticipate and 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 apply Argonne techniques, technologies, tools, and training to foster the creation of high-wage jobs, to ease urban blight, and to support the renovation of urban infrastructure.
- Find opportunities to apply our special capabilities beyond DOE, so as 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 cooperative 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, Argonne has considerable strength and breadth of expertise in scientific and technical areas related to energy and the environment, and we are organized to integrate multidisciplinary capabilities in research, development, and demonstration of new technologies. Application of these capabilities has allowed us to develop solutions to a wide variety of real-world problems and to 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 — including 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 for computing and communications.

Resources that can be applied beneficially to this initiative are described in Table IV.7. 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.7 Science and Technology for Environmental Stewardship** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs							
Operating	10.0	13.0	15.0	17.0	19.0	19.5	22.0
Capital Equipment	0.4	0.5	0.5	0.5	0.5	0.5	0.5
Construction	-	-	-	-	-	-	-
Total	10.4	13.5	15.5	17.5	19.5	20.0	22.5
Direct Personnel	32.0	39.0	40.0	41.0	42.0	43.0	44.0

## 6. 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., via 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 non-defense applications that use biochips to detect nucleic acids, peptides, and proteins. Current spin-off 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.8. The funding increase for FY 2005 is sought from DOE, other federal agencies, and the private sector.

**Table IV.8 Integrated Biodefense Systems**  
(\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs							
Operating	3.0	3.5	3.5	3.5	3.5	3.5	3.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	3.0	3.5	3.5	3.5	3.5	3.5	3.5
Direct Personnel	6.5	7.0	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.9. Funding is sought from DOE-Energy Efficiency and Renewable Energy (ED), DOE-Fossil Energy (AA), other federal agencies, and industrial partners.

**Table IV.9 Biobased Products** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
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

**C. National Security**

As Secretary Abraham has said, national security is DOE’s overarching mission. It is also one of the four traditional underlying DOE mission areas.

**1. Nuclear National Security**

*Situation*

Our current work on nuclear national security aims to reduce threats posed by nuclear and radiological materials and the illicit or improper use of nuclear and radiological facilities. 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 of detecting, monitoring, tracking, and limiting the spread of weapons of mass destruction and also the spread of radiological materials that, if used in weapons, could cause widespread disruption and impose large costs. A related focus is on the safe and proper use of nuclear energy and nuclear research facilities.

Among the most pressing problems facing the United States is the breakdown of systems for controlling nuclear materials in the independent countries of the former Soviet Union (FSU). The United States, with several other nations, is providing technical assistance to help independent FSU countries improve their accountability and control systems.

Another major concern is radiological materials throughout the world, for which only limited accountability and controls are in place. The United States is again one of several countries providing technical assistance to improve security and controls.

Argonne's nuclear national security program, with an annual budget totaling approximately \$38 million, includes several significant components:

- The Reduced Enrichment for Research and Test Reactors (RERTR) program develops new fuels, targets, and analysis methods to enable research reactors throughout the world to operate with low-enrichment uranium instead of highly enriched uranium in their fuel and targets.
- The Material Protection Control and Accounting (MPC&A) program assists nuclear facilities in Russia and the independent FSU countries by offering surveys of the current status of protection and accounting for nuclear materials, recommendations for improvements, and coordination of upgrade plans and their implementation. This program includes training courses, offered both at Argonne and abroad, that enable foreign specialists to use new security and accounting systems effectively.
- The Verification Technology program develops sensitive, selective instruments to detect radiation and chemical and biological effluents that might indicate clandestine proliferation.
- The Nuclear Export Control program 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 export control systems in the independent FSU countries, supplier countries, and countries through which relevant materials and equipment are transported.
- The transportation and final storage of nuclear materials from the BN-350 breeder

reactor in Kazakhstan serves 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 serves U.S. nonproliferation goals by ensuring that the reactor can never again produce nuclear materials suitable for weapons. This program uses a unique organizational approach in which issues are addressed by integrating design teams representing various Kazakh organizations and Argonne.
- The joint U.S.-Russian materials disposition program 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 Implementation program 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) program uses a proven model for achieving technology commercialization through partnerships among U.S. industry, U.S. national laboratories, and former Soviet scientific institutes.
- The Radiological Threat Reduction Program helps to secure the radiological materials located abroad that pose the greatest risk to U.S. security, by means of visits by technical assessment teams comprising experts in physical security, materials control and accounting, and health physics.
- The Radiological Cleanup Program operates under a congressional directive to develop a national cleanup policy for response to incidents involving radiological dispersal devices or improved nuclear devices. Starting with evaluations of potential human health risks under various scenarios, we derive

cleanup criteria for real and personal properties.

- The national, multiagency Emergency Response Program addresses releases of oil and hazardous substances. We are developing integrated sampling strategies for emergency responses by using approaches developed for our Adaptive Sampling and Analysis Program, an expedited approach to collecting data for characterizing and remediating hazardous waste sites.

### *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. We promote the safe, secure, and transparent operation of nuclear and radiological facilities around the globe and help to implement associated U.S. policy initiatives.

### *Issues and Strategies*

We plan to integrate and increase our support for U.S. nuclear national security initiatives, particularly by exploiting our unique expertise in nuclear and sensor technologies. Activities of the RERTR program 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 radioisotope, by using low-enrichment uranium instead of highly enriched uranium. Our expertise will also be used to enhance the security of nuclear materials at additional sites in the independent FSU countries, as well as to reduce the availability of weapons-usable materials by decreasing 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 the NNSA's and other federal agencies' 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 independent FSU countries.

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 and monitoring. 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 if the nation is to plan adequately for new potential targets, different modes of delivery, different weapons, and different consequences, including functional defeat of critical economic infrastructures and processes. Systems for responding to actual events must also evolve.

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

1. Nonproliferation Technologies
2. Nuclear Fuel Cycle Technology Applications
3. Training for Specialists in Nuclear Material Protection and Law Enforcement
4. Global Threat Reduction

### ***Initiative: Nonproliferation Technologies***

We propose significant expansion of our activities related to the development, demonstration, and deployment of nuclear material safeguards and process-monitoring technologies. For the 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 to 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 propose in addition to help develop detectors for discerning the movements of radiological dispersion devices and to assist in 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 the NNSA (NN), DOE-EM (EW), and DOD. See Table IV.10.

**Table IV.10 Nonproliferation Technologies**  
(\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
<b>Costs</b>							
Operating	4.5	5.0	6.0	6.0	6.0	6.0	6.0
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	4.5	5.0	6.0	6.0	6.0	6.0	6.0
Direct Personnel	10.0	11.0	12.0	12.0	12.0	12.0	12.0

#### ***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, to promoting the safe and secure operation of nuclear and radiological facilities, 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 observability and transparency for the facilities of all International Atomic Energy Agency (IAEA) member states that do not already possess nuclear weapons. Designing fuel cycle processes and operations from the beginning 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 answer 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.11.

**Table IV.11 Nuclear Fuel Cycle Technology Applications** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
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	11.5	12.0	12.5	12.5	12.5	12.5	12.5

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

For several years we have supported the MPC&A program of the NNSA by providing training to nuclear security personnel from Russia and the independent FSU countries. In coming years we will offer to expand the number of classes conducted, thereby enabling the 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.12. Funding will be sought from DOE-Defense Nuclear Nonproliferation (NN).

**Table IV.12 Training for Specialists in Nuclear Material Protection and Law Enforcement** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FT10
Costs							
Operating	3.0	2.5	2.5	2.5	2.5	2.5	2.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	3.0	2.5	2.5	2.5	2.5	2.5	2.5
Direct Personnel	6.0	5.0	5.0	5.0	5.0	5.0	5.0

***Initiative: Global Threat Reduction***

In May 2004, Secretary Abraham announced DOE’s Global Threat Reduction Initiative (GTRI), a new phase in the global nonproliferation effort responding to the threat of misuse of nuclear and radiological materials by terrorists. Broadly speaking, the GTRI will consolidate and accelerate existing threat reduction programs and will add a substantial new effort to remove, secure, relocate, or dispose of weapons-usable and radiological materials that are not included in existing threat reduction programs, in a comprehensive and expeditious manner.

The GTRI will incorporate Argonne’s key ongoing contributions to programs developing high-density low-enrichment-uranium fuels and converting research reactors worldwide to these new fuels. For all existing programs being included in the GTRI, the central goals are (1) to work in partnership with Russia to repatriate all fresh and spent nuclear fuel that originated in Russia but now is at research reactors around the world, (2) to complete — on an accelerated schedule — the repatriation from research reactors of spent high-enrichment-uranium fuel that originated in the United States, and (3) to complete the conversion of civilian research reactors from high-enrichment-uranium fuel to low-enrichment-uranium fuel. The major new component of the GTRI involves securing, removing, relocating, or disposing of nuclear and radiological materials and related equipment that are not covered by existing threat reduction programs. Extensive international cooperation and collaboration will be necessary to establish an effective nonproliferation regime in this arena, particularly for materials that did not originate in Russia or the United States or that are located in countries posing challenges that the United States and Russia cannot address alone.

The NNSA has established a new unified organization with the sole purpose of achieving the GTRI’s objectives. Plans call for more than \$450 million to be dedicated to these efforts over the next decade. Building on its work on low-enrichment-uranium research reactor fuels and conversion analyses, Argonne is well positioned to play a leading role in new threat reduction efforts. Future editions of this *Institutional Plan* will provide specifics.

## 2. Homeland Security

### *Situation*

Argonne's homeland security programs addressing infrastructure assurance and counterterrorism are leading to broader recognition within the Department of Homeland Security (DHS) of the Laboratory's capabilities. The overall aim of our current work is to assure the security and reliability of critical U.S. infrastructures and other key national assets that are threatened by disruptions resulting from natural events, accidents, or deliberate acts such as terrorist attacks — and to assure the safety of associated populations. This work addresses physical and 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 plan for the Nuclear National Security area in Section IV.C.1). Work to increase homeland security directly supports both DOE's overarching national security mission and the DHS mission.

Our work on infrastructure assurance and counterterrorism draws on expertise, knowledge, technologies, and specialized research facilities developed over decades for other DOE missions and for non-DOE sponsors. By leveraging our core science and technology competencies, Argonne's 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 \$25 million. Significant components of these programs include the following:

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

disruptions and system behavior, as well as 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 disruptions.

- 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 infrastructures (e.g., the infrastructure 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 infrastructures deemed to be at above-average risk, such as subways, airports, and public buildings.
- Various smaller Laboratory projects are emerging to deal with threats in the transportation and agricultural sectors posed by weapons of mass destruction and weapons employing radiological materials.

In addition to these programs, 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 risks 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 that can 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 at the contaminated site for rapid turnaround, and the mobile facility can confirm decontamination after cleanup operations.
- The Dilute Chemical Agent Facility on Argonne's Illinois campus, 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. It 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 above 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 and weapons employing radiological materials.

#### *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 molecular biology, structural analysis, radiation chemistry and photochemistry, catalysis and electrochemistry, and chemical and biological decontamination. For example, a microchip-type sensor that isolates and labels 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 propose 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 include two entities funded by the NIH: 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. Altogether, more than 100 scientists are involved. The RBL will provide RCE researchers with facilities certified to "biosafety level 3" (the third highest of four levels). See Section S1.C in Supplement 1 for further information.

A high-priority initiative for Argonne is enlargement of its capabilities to handle classified materials, information exchanges, and meetings. These increased capabilities will be important not only for research to improve infrastructure assurance, but also for research serving other DOE missions, through such programs as the Highly Enriched Uranium Transparency Implementation program.

Argonne will continue to work with other laboratories, government agencies, universities, and the private sector, as well as with various first-responder communities, to reduce the risks posed by terrorists and other potentially devastating threats. The Laboratory will particularly seek ways to reduce threats from the hostile use of various specialized materials. We will also seek to help local, state, and federal officials respond to emergencies by using the broad range of our scientific and technical facilities.

***Initiative: Homeland Security —  
Infrastructure Assurance  
and Counterterrorism***

We propose to expand our current R&D 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. infrastructures (including cyber-based information systems) and associated populations from disruption and (2) will, where disruptions do occur, 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 specifying 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 Commerce Department's 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 of these areas to address the unprecedented range of physical and cyber threats to critical U.S. infrastructures from natural causes, accidents, and deliberate acts such as the 2001 terrorist attacks on the World Trade Center and the 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 in 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 Homeland Security — Infrastructure Assurance and Counterterrorism** (\$ in millions BA, personnel in FTE)

	FY04	FY05	FY06	FY07	FY08	FY09	FY10
<i>Costs</i>							
Operating	19.9	24.9	24.9	24.9	24.9	24.9	24.9
Capital Equipment	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Construction	-	-	-	-	-	-	-
Total	20.0	25.0	25.0	25.0	25.0	25.0	25.0
Direct Personnel	80.0	100.0	100.0	100.0	100.0	100.0	100.0

### 3. National Defense

#### *Situation*

In conjunction with its work to enhance homeland security, Argonne is also working to apply similar technologies and processes to serve the national defense more broadly.

One important area of work involves applying the Laboratory’s very extensive, highly specialized knowledge of radiological materials to equip first responders with the knowledge and instrumentation they need to deal with such materials. In general, Argonne is a major national resource in its broad understanding of materials, materials detection, and materials handling.

Another important area of work involves attribution and forensics for radiological materials used in attacks. The Laboratory is currently developing a database that will help defense agencies perform these crucial functions.

#### *Mission*

Argonne will apply its technical and analytical expertise, resources, and facilities — in the physical, biological, and computational sciences and in technology — to help the nation’s defense agencies pursue their missions to reduce risks to U.S. interests resulting from terrorism and other threats.

#### *Issues and Strategies*

Argonne has technical capabilities in research areas that are highly relevant to the missions of the defense agencies, notably in 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; infrastructure analysis and systems analysis; and logistics systems analysis. We can also provide technical support for various

rapid response functions related to the missions of defense agencies.

We will continue to explore opportunities to leverage our ongoing R&D and demonstrations to enhance the defense of the nation and its interests, by working with the federal agencies responsible for that vital mission. See Section S1.B in Supplement 1 for a description of our current work for various DOD agencies.

## D. Collaborative R&D Partnerships

### *Situation*

For Argonne's research to have an impact and provide benefits, results must be readily accessible to commercial firms for further development and applications that meet the needs of industry and the public. We pursue these objectives through broad publication of results, development and licensing of patent portfolios, and partnering with industry. Our research partnerships with industry and academe 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 jointly held 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, academe, and other not-for-profit organizations, in order to provide competitive benefits to users of Argonne technologies and, ultimately, enhanced energy security, national security, and environmental quality for the nation.

### *Mission and Vision*

The mission and vision of Argonne's technology transfer program includes five major elements:

- Enhance the competitiveness of U.S. industry by transferring Argonne technology

solutions to industry and engaging in 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.
- Increase interchange and expand joint efforts with the University of Chicago and other midwestern universities through the Midwestern Research University Forum.

### *Approach*

We use a variety of tactical approaches to accomplish our technology transfer mission and provide benefits to the nation. Most importantly, we pursue numerous cooperative R&D agreements (CRADAs) through joint industry-Laboratory research programs. Increasingly, we use reimbursable work-for-others contracts as a vehicle for industrial agreements and transfer of our technologies. In addition, we use "full funds-in CRADAs" as a basis for developing cooperative research partnerships that move Laboratory technologies toward commercialization. In FY 2003 Argonne initiated a joint program with the University of Chicago to first 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. Over the past year we made significant progress toward developing appropriate policies and approaches for obtaining funding.

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

## E. 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.

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 Energy Systems, and Hydrogen Research and Development.

Several LDRD projects will be supported under 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. This upper limit generally approximates 4.5% to 5.0% of our projected total of operating and equipment funding.



# V. Operations and Infrastructure

## Strategic Plan

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Our fourth strategic objective is stated in Chapter II: “The University of Chicago and Argonne will continuously improve the cost-effectiveness, management, and operations of the Laboratory.” This chapter presents strategic plans for the following areas of operations and infrastructure at Argonne: human capital; site and facilities; environment, safety, and health; integrated safeguards and security management; information management; communications, outreach, and community relations; and performance management. The chapter begins with general statements of mission, situation, and goals and strategies for operations and infrastructure.

### *General Mission*

Operations infrastructure and support activities are crucial to the effective and efficient achievement of our R&D mission. Operations organizations work as partners with Argonne’s R&D programs, providing cost-effective, customer-focused infrastructure and services that enable the creation of world-class science, technology, and service products.

### *General Situation Analysis*

Because operations and infrastructure are funded as a charge to the total program funding we receive, there is always great incentive to reduce these overhead costs while still maintaining the effectiveness and quality of operations and services. Every overhead dollar saved is an additional dollar for direct funding of research programs.

### *General Goals and Strategies*

Management of our operations infrastructure and support functions has seven broad goals, specified below along with strategies for their achievement:

- Enable and support Argonne’s R&D work. Provide efficient services, business processes, and information systems that are responsive to programmatic requirements and initiatives.
- Deliver distinctive customer service. Provide efficient customer-focused services that improve employee productivity, advance programmatic goals, and drive operational excellence.
- Provide exceptional infrastructure. Develop innovative strategies for building and maintaining highly reliable, cost-effective site utilities and facilities that support world-class science and technology.
- Enhance external and internal communication. Increase national recognition of our contributions to science and technology. Encourage sharing of information and ideas among all employees. Expand productive partnerships.
- Demonstrate success in safety and security. Effectively integrate safety and security into all operations, perform favorably compared to national standards and external peers, and continually improve performance. Provide appropriate access to Argonne and its user facilities through implementation of carefully considered policies and requirements for both safety and security.
- Promote Argonne as an employer of choice. Provide a high-quality work environment and competitive salary and benefits — all highly valued by employees.
- Deliver outstanding performance. Earn outstanding ratings from DOE in all contractual performance areas for Laboratory operations. Meet the exacting standards of the University of Chicago’s peer review process.

The cornerstone of our approach to efficient operations and successful research is integration of safety, security, environmental, and other

operational responsibilities and activities into line management and work practices throughout the Laboratory, at all levels. Our Integrated Management program addresses the full range of relevant risks we face in our work. It encompasses our Integrated Safety Management program, our Integrated Safeguards and Security Management program, and our Environmental Management System. In all areas, Integrated Management involves careful attention to the following five steps: (1) define the scope of work, (2) analyze the risks, (3) develop and implement controls, (4) work within the controls, and (5) use feedback and make improvements. Policy formulation, leadership, and coordination are provided by the Environment, Safety, Security, and Health Committee. In addition, security considerations are included in assessments of performance of line management and in oversight conducted by the office for Environment, Safety, and Health/Quality Assurance Oversight.

We continually strive to increase the efficiency of our operations and support units while maintaining their effectiveness and quality. The performance-based contract between the University of Chicago and DOE, hereafter referred to as the *Prime Contract*, provides a system for encouraging continuous improvement in our operational functions (as discussed further in Section V.G). With collaboration and support from DOE's Chicago Operations and Argonne Site Offices, we continually strive to refine a full range of best business practices.

## A. Human Capital

### *Situation*

The quality of technical staff is a primary determinant of the performance of an R&D laboratory. Our human resources strategy is designed to develop strong leadership, to support a creative and diverse workforce, and to recruit and develop the talent needed to implement the Laboratory's programmatic activities and initiatives.

Human resources management at Argonne is conducted as a partnership between our programmatic and operations organizations and

the central Human Resources Division. Critical to the success of this effort is a focus on Laboratory policies, programs, and initiatives that influence an individual's decision to join the Laboratory, that help shape the working environment for those making a career at Argonne, that contribute to the well-being of employees (even after they retire) through benefits such as health insurance and retirement income, and that comply with federal and state regulations.

Total commitment to equal opportunity for all people is a fundamental Laboratory policy. Argonne values the diverse cultural and ethnic backgrounds of its employees and strives to create an environment that capitalizes on these differences as one means of maintaining a high-performance workforce.

### *Goals*

The goal of Argonne's human capital management is to support the strategic objectives of its programmatic and operations organizations by developing and implementing programs that attract, develop, compensate, and help to retain a qualified and diverse staff. Specific objectives include the following:

- Directly link and integrate centralized human resources strategies with the strategic needs of division managers.
- Improve the quality of the employee's work life in order to foster job satisfaction, individual contributions to Laboratory performance, and organizational effectiveness.
- Maintain a compensation policy that is competitive with policies at peer organizations and that rewards superior performance.
- Promote the commitment of managers at all levels to equal opportunity, affirmative action, and diversity.
- Develop Laboratory leadership and staff capabilities through targeted management training and skill development opportunities.
- Provide services that promote the well-being and productivity of Argonne employees.

### Strategies

The key to effectively integrating centralized human resources strategies with the needs of individual programmatic and operations divisions is frequent dialogue with division managers, particularly regarding opportunities for centralized services beyond purely administrative functions. To achieve this integration, Human Resources uses formal management surveys, input from liaisons within other divisions, and direct dialogue with division managers. During regularly scheduled one-on-one meetings, division directors and human resources representatives discuss personnel and recruitment needs, training, diversity targets, and the division's general human capital needs.

Achievement of Laboratory goals requires top-quality staff who find personal and professional fulfillment in their work. (Table V.1 describes their extensive academic training.) Our success in employing high-caliber staff starts with recruiting the best and the brightest, including people from diverse backgrounds. In FY 2003 Argonne recruiters participated in nine job fairs, through which they made direct contact with more than 900 potential new hires.

**Table V.1 Academic Degrees of Argonne Staff<sup>a</sup>**

Occupational Category	Total	PhD	MS/MA	BS/BA	Other <sup>b</sup>
Officials and Managers	535	248	141	105	41
Scientists	656	317	126	139	74
Engineers	519	195	135	130	59
Managers and Administrators	293	23	51	107	112
Technicians	459	0	4	58	397
All Others	955	0	5	57	893
<b>Grand Total</b>	<b>3,417</b>	<b>783</b>	<b>462</b>	<b>596</b>	<b>1,576</b>

<sup>a</sup> Number of full- and part-time regular employees as of September 30, 2003.

<sup>b</sup> Associate level degree or less.

We are committed to strengthening the vitality, quality, and diversity of our workforce. Maintenance of a competitive compensation structure is important in our competition for critical talent. We manage all components of compensation — base pay, merit increases, compensation supplements, and promotion-related increases — as a coordinated whole. Each

employee's compensation (apart from fringe benefits) is linked to achieved performance, as evaluated under our appraisal process. That process focuses on sustained performance and compensation relative to peers and to the external market.

Argonne's Performance Evaluation Process committee recently enhanced the Laboratory's performance appraisal process through introduction of a new online appraisal form that focuses on establishing clear connections between the goals of each employee, the goals of the Laboratory, and the goals of intermediate levels of management. At the same time, we provided performance management training for 1,039 participants and developed online training to assist supervisors in writing performance appraisals and conducting interim discussions with employees about development.

Total commitment to equal opportunity for all people is a fundamental Argonne policy. Our annual *Affirmative Action Plan* gives managers a summary of accomplishments and a blueprint for the future. Supervisors are held accountable for progress in this area. In 2003 we received DOE's Equal Employment Opportunity and Diversity Best Practices Award for our career development workshops on "Survival Skills for Successful Women Scientists and Engineers." We also established a Diversity Council that recommends to the laboratory director strategies for fostering an inclusive environment in which all members of our diverse workforce can excel and contribute to Argonne's success. Table V.2 describes the Laboratory's current employee populations.

We supplement the formal education of our employees with performance-enhancing training. Course offerings are based on both assessment of professional development needs and compliance with DOE directives. The wide range of subjects offered includes supervisory skills, team building, project management, presentation skills, and R&D proposal development. Argonne's emphasis on employee learning and development was acknowledged in 2003 by receipt of the prestigious Workforce Chicago 2.0 Award. Mayor Richard Daley presided over the awards ceremony, which recognized Argonne's commitment to integrating employee development strategies into the Laboratory's goals and operation.

**Table V.2 Equal Employment Opportunity at Argonne<sup>a</sup>**

Occupational Category	Total		Minority Total		White			
	Male	Female	Male	Female	Male	Female		
Officials and Managers	447	88	38	9	409	79		
Scientists and Engineers	1,001	174	152	33	849	141		
Managers and Administrators	118	175	6	26	112	149		
Technicians	408	51	43	8	365	43		
Clerical Workers	28	400	5	66	23	334		
Craftsmen and Laborers	324	38	60	17	264	21		
Service Workers	129	36	29	10	100	26		
<b>Totals</b>	<b>2,455</b>	<b>962</b>	<b>333</b>	<b>169</b>	<b>2,122</b>	<b>793</b>		

Occupational Category	African-American		Hispanic		Native American		Asian	
	Male	Female	Male	Female	Male	Female	Male	Female
Officials and Managers	3	3	6	2	0	0	29	4
Scientists and Engineers	16	1	12	4	3	0	121	28
Managers and Administrators	1	11	2	6	1	0	2	9
Technicians	17	1	16	1	2	1	8	5
Clerical Workers	2	29	3	24	0	1	0	12
Craftsmen and Laborers	43	12	13	4	1	1	3	0
Service Workers	19	6	4	3	2	1	4	0
<b>Totals</b>	<b>101</b>	<b>63</b>	<b>56</b>	<b>44</b>	<b>9</b>	<b>4</b>	<b>167</b>	<b>58</b>

<sup>a</sup> Includes both full-time and part-time regular employees as of September 30, 2003.

Additional Argonne efforts to promote the well-being and productivity of employees include programs on health screening and wellness, financial education, and dealing with life and family issues. Examples are workshops on estate planning and preretirement planning, a women's wellness series featuring seminars and health screenings, an interactive roundtable on elder care, and a health fair.

To increase the effectiveness and quality of human resources information and to reduce costs, we use electronic approaches to information management and reduce our dependence on traditional paper documents. For example, we (1) created ResBuilder, an improved online tool that enables external candidates to submit resumes through the Argonne web site, (2) implemented a process for scanning past performance appraisals into an electronically accessible format, and (3) created an electronic database of past conflict-of-interest forms. Our intranet provides electronic versions of policy and procedures manuals related to human resources, benefit plan descriptions, and information on the historical performance of retirement funds.

## B. Site and Facilities

### 1. Argonne-East

#### *Situation*

Argonne conducts basic and technology-directed research at two sites owned by DOE. Argonne-West, which will be incorporated into the new Idaho National Laboratory in FY 2005, is discussed separately below.

Argonne-East is located on a 1,500-acre site in DuPage County, Illinois, about 25 miles southwest of Chicago. The physical infrastructure at Argonne-East contains 4.8 million square feet of floor space, including 77 thousand square feet of nearby leased space. The facilities, valued at approximately \$1.9 billion, currently accommodate about 4,800 persons (including DOE employees, contractors, and guests). Throughout the year, over 2,000 other researchers use the Laboratory's scientific facilities as visitors or collaborators. Argonne-East facilities are nearly 99% occupied.

*Vision*

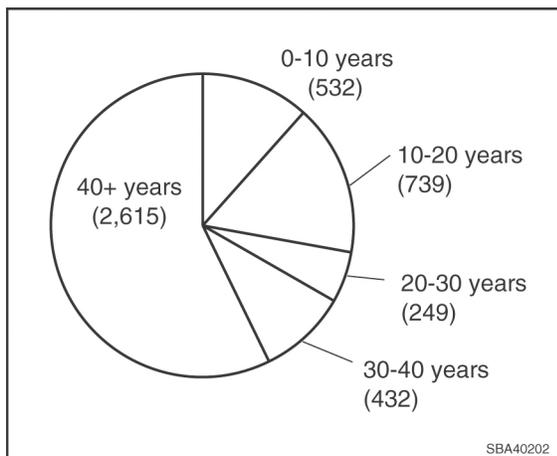
Argonne will retool its physical setting to achieve a 21st century infrastructure having appropriately configured research facilities that provide reliable, safe, secure, efficient, attractive working environments suitable for world-class science, engineering, and technical services.

*Issues and Strategies*

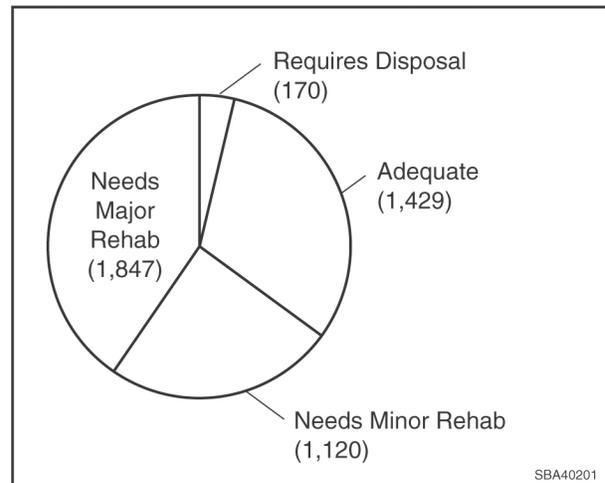
In the area of site and facilities, the principal challenges Argonne is addressing are the normal aging of buildings and infrastructure and a substantial need for upgraded laboratory facilities to meet the challenges of the 21st century. As Figure V.1 shows, 58% of Argonne-East facilities are over 40 years old.

In recent years Argonne-East has made substantial progress toward the rehabilitation and replacement of its facilities. However, as Figure V.2 shows, an estimated 40% of the site’s occupied facilities are still in need of major rehabilitation or upgrades. Thirty-one percent of the facilities are considered to be in adequate condition, while approximately 4% of floor space is in substandard facilities that require disposal. Most of this last category (87,500 square feet) is presently surplus and does not need replacement.

Over the infrastructure planning horizon, new programmatic facilities are likely to expand the



**Figure V.1 Age of Argonne-East Facilities (values in thousands of gross square feet)**



**Figure V.2 Condition of Argonne-East Facilities (values in thousands of gross square feet)**

base of modern, efficient space at Argonne-East. Nevertheless, substantial need for rehabilitation of older facilities will remain.

Strategic modernization of Argonne-East facilities centers on three coordinated, phased upgrade projects addressing (1) building electrical systems, (2) building mechanical and control systems, and (3) laboratory space upgrades. The work scope of each project phase is based on priorities established through the Laboratory’s Condition Assessment Survey process.

In general, Argonne-East upgrades a building’s electrical system to support greater mechanical and functional power and lighting loads and to allow more extensive use of equipment. Improved mechanical and control equipment and upgraded mechanical, distribution, and collection systems are installed as the basis for a building utility support network that is more flexible and adaptable.

In coordination with these efforts, Argonne-East plans significant upgrades to laboratory and office spaces to bring them to today’s standards. Modernization is planned for 12 buildings providing 2 million gross square feet of space. The site’s new central supply facility exemplifies application of the principles of sustainable design and facilities integration, which will be a hallmark of planned infrastructure upgrades.

Roof replacement is a major Argonne-East initiative as the roofs of major buildings near the end of their 20-year design life and the frequency of repairs increases. Similarly, deteriorating roads and parking lots will require substantial investment over the next 5 years.

Other site improvements also have high priority. The proposed Phase V Fire Safety Improvements project will reduce the potential for property loss. In addition, the site's central heating plant will require a major upgrade of its auxiliary systems and equipment by FY 2008.

To achieve the 21st century infrastructure documented in the Laboratory's *FY 2002 Strategic Facilities Plan*, Argonne-East requires capital funds totaling approximately \$275 million through FY 2010. In addition, the site requires a total of \$58 million in direct operational funding from the DOE Office of Science to undertake needed environmental and demolition work not currently supported by funding from the DOE Environmental Management program.

Increased reliance on the use of internal operating funds to address deferred maintenance and to provide additional means of recapitalizing Laboratory infrastructure have been identified as DOE priorities. The goal of the Office of Science is to increase the level of maintenance supported by operating funding from the historical rate of approximately 1% of replacement plant value to 1.4% in FY 2004 and 2% thereafter. The 2% goal will be a significant challenge. Moreover, recent DOE guidance specifies no Science Laboratories Infrastructure program line-item project funding through FY 2010. Elimination of this support will make reducing deferred maintenance and modernizing infrastructure exceedingly difficult. To provide facilities for new scientific initiatives, the Laboratory has increasingly turned to the state of Illinois and to other third-party financing.

## 2. Argonne-West

### *Situation*

Argonne-West is located on an 800-acre tract within the Idaho National Engineering and Environmental Laboratory (INEEL), about

35 miles west of Idaho Falls, Idaho. Argonne-West is devoted mainly to R&D on nuclear technologies and nuclear environmental management.

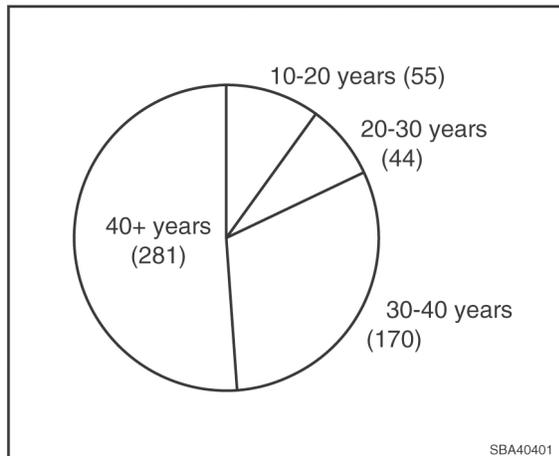
Argonne-West contains 550,000 square feet of floor space, with an estimated replacement value of \$380 million. The current site population is about 640 persons. Recent renovations and continuing maintenance of major facilities are enabling Argonne-West to pursue important research on nuclear technology for DOE. Program sponsors other than DOE-Nuclear Energy are charged for facility utilization in a manner similar to the space use charge-back system at Argonne-East. Site services such as fire protection and dosimetry are purchased from the site contractor for INEEL.

### *Issues and Strategies*

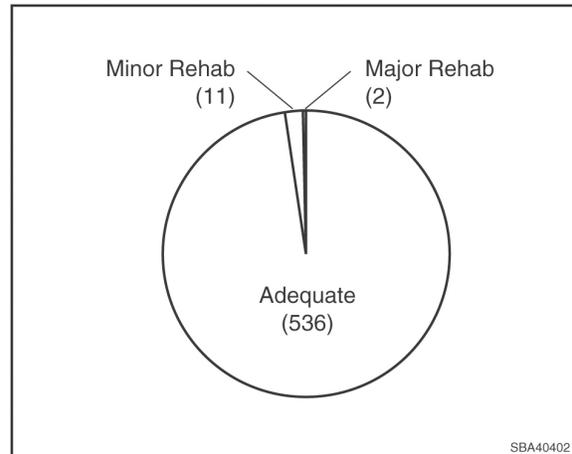
In February 2004, DOE released a draft request for proposals to establish a new national laboratory to be called Idaho National Laboratory (INL). The new INL will combine Argonne-West with INEEL. In announcing the request for proposals, Secretary of Energy Abraham stated that "the new Idaho National Laboratory will be the epicenter of our efforts to expand the use of nuclear energy as a reliable, affordable, and clean energy source for our nation's energy future and establish opportunities for Idaho businesses, its people, and universities. The technologies that will be born at this lab will help us realize our far-reaching energy and environmental goals of reducing dependency on foreign sources of energy, while still allowing for vibrant economic growth."

This shift in institutional alignment creates both opportunities and challenges. The central opportunity is to expand nuclear power research, both within the new laboratory and at Argonne in association with INL. The immediate challenge is to restructure Argonne's management and operations so that the two separate entities thrive, with strong ties for cooperative R&D.

In the area of site and facilities, Argonne-West also faces challenges from the normal aging of buildings and infrastructure and a substantial need for upgraded laboratory facilities. As Figure V.3



**Figure V.3 Age of Argonne-West Facilities (values in thousands of gross square feet)**



**Figure V.4 Condition of Argonne-West Facilities (values in thousands of gross square feet)**

shows, 82% of space at Argonne-West is over 30 years old. Diligent maintenance, however, has kept the facilities in generally good condition (Figure V.4).

Strategic modernization of Argonne-West facilities focuses on upgrading sitewide utilities and support equipment and on maintaining major nuclear and radiological facilities to support a comprehensive nuclear power R&D mission. The transition to the INL will require reconsideration of infrastructure priorities at Argonne-West and INEEL. This reconsideration started in 2003 with joint preparation of a ten-year site plan.

Roof replacement is a major Argonne-West need, as the roofs of major buildings approach the end of their design life and the frequency of repairs increases. Similarly, deteriorating sidewalks will require substantial investment over the next five years.

The Experimental Breeder Reactor-II (EBR-II) Plant Closure Project, successfully completed in FY 2002, placed the facility in a safe, stable condition requiring minimal surveillance and maintenance. Under the RCRA (Resource Conservation and Recovery Act) Part B Permit for EBR-II issued by the state of Idaho in December 2002, DOE-Nuclear Energy must complete "RCRA clean closure." Funding in FY 2004 is supporting development of a preliminary cost and schedule baseline.

The demand for hot cell and laboratory space is expected to be particularly high for INL. A major focus is providing the facilities and infrastructure needed to deal with spent fuel and nuclear waste (for the Advanced Fuel Cycle Initiative program, for example).

Argonne-West is planning construction of the Remote Treatment Project Facility, a \$90 million major hot cell facility needed to handle and process for disposal remotely handled mixed transuranic waste from both Argonne-West and INEEL. Disposal of this waste outside Idaho by the year 2018 is required by the court-ordered settlement agreement between DOE and the state of Idaho. Moreover, after 2018 this facility will be a cornerstone — along with the Hot Fuel Examination Facility and the Fuel Conditioning Facility — for a much needed DOE hot cell center that will (1) develop base technologies to address problems associated with disposal of remotely handled waste and (2) support research to improve nuclear fuels and materials.

## C. Environment, Safety, and Health

### *Situation*

Protection of the environment, safety, and health (ES&H) is a fundamental value for Argonne. Safety statistics confirm that the

Laboratory is a safe place to work, and both analysis and experience indicate that our operations have minimal environmental impact. Our FY 2003 *Self Assessment* explains our progress in ES&H in detail (URL: [www.ipd.anl.gov/cpmr/text.html](http://www.ipd.anl.gov/cpmr/text.html)).

We recognize the need for continuous evaluation and improvement in our ES&H programs, and we have firmly embraced Integrated Safety Management (ISM) policy as an operating philosophy. ISM maintains employee attention to essential ES&H issues, goals, and ideas. The structure of our ES&H program is described in depth in the *Integrated Safety Management (ISM) Program Description, Revision 7*, dated March 19, 2003 (URL: [http://www.anl.gov/ESH/main/ism/pdf/ISM\\_rev7.pdf](http://www.anl.gov/ESH/main/ism/pdf/ISM_rev7.pdf)).

Our ISM program includes investigation of incidents and proactive management of Worker's Compensation claims through coordination of (1) medical department interventions and ES&H analyses with (2) investigations of causes by line managers. The central goal is to protect employees from occupationally related injury or illness.

Our medical department supports DOE's Beryllium Worker Protection Program and offers beryllium blood lymphocyte testing to voluntarily participating employees. In cooperation with DOE, we assist the Oak Ridge Institute for Science and Education (ORISE) in offering former employees an opportunity to participate in ORISE's Beryllium Medical Surveillance Program. Argonne strongly supports both of these beryllium-related programs.

We actively support the Energy Employees Occupational Illness Compensation Program Act (EEOICPA) of 2000 by supplying employment, exposure, and medical records to the Department of Labor, the National Institute for Occupational Safety and Health, and the DOE Office of Worker Advocacy, in response to EEOICPA inquiries. We handled 298 requests in 2002 and 154 in 2003.

#### *Goals and Objectives*

The overall goal of our ES&H program is to ensure that all activities are conducted (1) with minimal and measured adverse impacts to

personnel and the environment and (2) within regulatory constraints. The central tenet of ISM throughout Argonne is line management responsibility and accountability, in conjunction with the expectation that each worker is involved in ISM and accepts responsibility for implementing and promoting it.

To strive for continuous improvement in achieving this overall goal, we have established five specific strategic objectives:

- Pursue "star status" under the DOE Voluntary Protection Program (VPP). The VPP will evaluate how well our ES&H program supports R&D activities and whether it is judged to be "outstanding" by both DOE and peer laboratories.
- Before the end of FY 2005, correct all deficiencies identified in FY 2003 by an Occupational Safety and Health Administration (OSHA) review team.
- Promote assessment planning by each major research and support organization, and ensure that their assessment plans include the proper mix of self-assessment and independent assessment to appropriately address the broad range of relevant ES&H issues.
- Establish and track appropriate indicators of ES&H performance that help promote improvements to the Laboratory's safety culture and research performance.
- Continue to implement and improve our environmental management system, continue to work toward good relations with stakeholders and surrounding communities, and maintain a long-term stewardship program for environmental monitoring of Laboratory sites.

#### *Strategies*

We regularly (1) evaluate our ES&H requirement documents to ensure that they reflect changing regulations, (2) implement the documented requirements, and (3) assess various ES&H program elements to measure implementation of requirements and to promote continuous improvement.

We use limited available resources to address ES&H concerns that pose the greater risks.

However, setting priorities often requires considerable judgment in such areas as promoting continuous improvement in the Laboratory's safety culture, in the performance metrics system, and in other ES&H systems. We rely on the creativity of our personnel to establish ES&H requirements and implementation strategies that are consistent with the risks presented by the work being done. Specific needs are documented as part of our *ES&H and Infrastructure (ESH&I) Management Plan* process.

We will continue to pursue our ES&H goals through our strategic objectives by using established systems operating pervasively under the ISM philosophy. We will continue to monitor our ES&H performance by using *Prime Contract* performance measures, other germane indicators, and our formal assessment program. We will continue to conduct frequent monitoring, surveillance, and evaluation in the workplace in order to implement specific ES&H performance measures and to address ES&H issues generally. We will continue to benchmark our processes and performance against those of other organizations.

We use a structured approach to ensure that facility conditions affecting ES&H are appropriately identified and prioritized among all our infrastructure needs. Our *ESH&I Management Plan* addresses required reporting to DOE by means of a detailed prioritization of all ESH&I projects. Projects related to ES&H include life safety and fire protection upgrades, environmental restoration, wetlands management, mechanical and control systems, an electrical service upgrade line item, decontamination and decommissioning activities, and a facility to store remotely handled transuranic waste for final disposal. More recently, we added projects to correct all of the deficiencies identified by an OSHA review team in FY 2003.

Our assessment program includes (1) assessments conducted by line organization managers to evaluate their own processes; (2) other self-assessments conducted by line organizations to evaluate specific topics; and (3) independent assessments conducted by Laboratory organizations or committees, by committees of the University of Chicago, by DOE,

or by other regulatory agencies or stakeholders. On the basis of the results of these assessments and other evaluations, we establish appropriate corrective action plans. Where corrective actions require significant resources and changes to the Laboratory infrastructure, we use the formal *ESH&I Management Plan* process to identify and prioritize resource allocation.

Through the Laboratory's Policies and Procedures system, we provide online access to more than 30 manuals related to ES&H. The system enables employees to view and print any manual and receive electronic mail notification when specified manuals are revised.

## D. Integrated Safeguards and Security Management

### *Situation*

Argonne has a responsibility to provide a safe, secure environment for its employees and visitors. Facilities, equipment, and information must be protected from theft, disruption, or misuse. Argonne-West protects significant quantities of special nuclear material. (Argonne-East possesses only small quantities of nuclear materials for limited research use.) Detection and prevention of electronic intrusion are among the more challenging aspects of security that we face.

Our mission predominantly involves fundamental research or technology development, with results disseminated openly and shared with the scientific community or made available to private industry. The quality of such work depends intrinsically on open dialogue and exchange of information. To serve our mission, each year we host thousands of foreign visitors and assignees, with whom we encourage active information exchange. We also participate in several officially sanctioned training programs with Russia, other countries of the former Soviet Union, and the International Atomic Energy Agency, as well as with the Department of Homeland Security. As a key player in leading-edge cooperative R&D with U.S. industry, we often conduct research involving vital commercial interests.

Most of our work is exempt from export regulation and is constrained only by prudent management to assure accuracy and proper disclosure. Nevertheless, certain Laboratory undertakings are subject to some combination of export control, classification, proprietary interest, and other restrictions on dissemination of results.

### *Objectives*

The Argonne-West Nuclear Program Services Division, the Argonne-East Security and Counterintelligence Division, and the Laboratory's chief information officer integrate their efforts to ensure the following results:

- Appropriate controls, systems, and security personnel protect special nuclear materials, classified matter, and high-value property against theft, diversion, or destruction.
- Site access controls provide a safe, secure working environment for employees; for guests; and for the large, diverse community of visiting researchers using Laboratory facilities.
- An active cyber security program makes electronic information freely and readily accessible to authorized users while protecting the information against disruption, compromise, destruction, or misuse.
- Appropriate processes and procedures are in place to assure controlled access to classified and proprietary information.
- Active awareness training and information programs educate all employees in how to maintain and enhance Laboratory security.

Argonne's security organizations work closely with each other and with senior management to ensure that policies and systems are optimized to protect Laboratory assets while enabling scientific progress.

### *Strategies*

In March 2004 Argonne-East combined its Office of Safeguards and Security and its Office of Counterintelligence. The new organization, the Security and Counterintelligence Division, is

expected to achieve a more effective, more coordinated approach to Laboratory security.

Protection of our physical assets requires a combination of access controls and other security measures. Protecting equipment, hardware, and materials at Argonne-East generally involves practices characteristic of industrial security. The protective forces at the Argonne-East site are trained security professionals who operate under contract to the Laboratory. Argonne manages and administers these forces, which include unarmed, trained security officers. The Laboratory is responsible for providing security for the entire Argonne-East site, including DOE offices and the New Brunswick Laboratory.

The larger quantities of special nuclear material at Argonne-West necessitate more extensive access controls and security force capabilities. The site's protective force is armed and certified by DOE to the SPO-II level. Some officers are certified to the SPO-III level and are assigned to special response teams. The site also employs physical protection systems such as sensors, alarms, physical barriers, entry control devices, and surveillance systems. An extensive, documented vulnerability analysis using DOE's updated *Design Basis Threat* has been completed.

Protection of intellectual property involves implementing an integrated network of policies, procedures, and practices. We meet all federal regulations related to national security and export control, including all applicable DOE regulations. Key to our program are access control and awareness training, supplemented by an extensive cyber security program for both classified and unclassified computing and by counterintelligence (CI) activities. A graded approach is used to determine the type and intensity of protective measures implemented.

Our cyber security program is designed to provide sophisticated, multitiered protection of both Laboratory sites from unauthorized access to information and disruption of information systems, with minimal disturbance of open scientific discourse. The program identifies information having national security interest; information whose distribution should be limited, from the perspective of Laboratory management, operations, and business activities; commercial or

proprietary information; and research information that has not yet been approved for release. Access to information that is not freely available to the general public is protected by graded or tiered access control mechanisms and is systematically monitored. Encryption is used where appropriate. Reporting and tracking capabilities are employed locally to anticipate cyber security problems before they occur, and a full response capability is maintained. Cyber security systems are evaluated and tested regularly, and improvements are deployed continuously to counteract changing threats. We provide computer security training to all our computer users.

After the terrorist attack on September 11, 2001, Argonne-East improved the site's physical security. Improvements evident to employees include the touching of badges when individuals enter the site, discontinuation of entry based solely on vehicle stickers, a larger protective force on duty, a requirement to wear identification badges at all times, a new joint operations center, and limitations on vehicle parking locations. Less evident are increased liaison with outside law enforcement authorities and regular notification about threats.

The DOE Office of Independent Oversight and Performance Assurance (DOE-OA) inspected the safeguards and security program and the cyber security program at Argonne-East in March and April 2003. The purpose was to evaluate the protection being provided for nuclear materials, classified matter, and sensitive unclassified information. DOE-OA reported that DOE and Argonne-East management have demonstrated strong commitment to the site's security program. Improvements in cyber security were considered particularly noteworthy, demonstrating an effective balance between security concerns and scientific productivity. All areas reviewed were determined to have achieved "effective performance."

We devote continuous effort to maintaining safeguards and security programs appropriate for the substantial quantities of special nuclear materials used and stored at Argonne-West. Recently upgraded were the central alarm system and the perimeter intrusion detection and

assessment system. In addition, we established a centralized location at the site for inspecting incoming freight.

The main objective of our CI program is to support DOE's CI program generally and the Laboratory specifically, by detecting, counteracting, and preventing political, economic, industrial, and military espionage and other clandestine intelligence-gathering activities directed at Argonne personnel, information, activities, facilities, and technologies. Our CI program is designed to deter and neutralize intelligence gathering on behalf of foreign governments or others. At both Argonne sites, this multifaceted program encompasses CI awareness, CI aspects of cyber security, CI-related investigations, and threat analysis, as well as liaison with federal, state, and local law enforcement and the U.S. intelligence community.

The CI program at each Argonne site supports and strengthens the Laboratory's overall safeguards and security program by working in concert with programs addressing security education and awareness, foreign visits and assignments, foreign travel, cyber security, operations security, information security, personnel security, nuclear material control and accounting, and physical security.

In October 2003 a team from the DOE Office of Counterintelligence conducted a two-week inspection of the Argonne-East CI program and gave it an overall rating of excellent. In more than 50 inspections dating back to 1999, the team had awarded that high rating only twice before.

## **E. Information Management**

Information management at Argonne emphasizes the effective development, communication, and management of scientific, technical, operational, and business information. Because of the broad importance of information management and its associated infrastructure, we manage those two intimately related areas both as integral parts of research programs and as institutional functions.

### *Vision*

We will maintain high-performance, cost-effective infrastructure and services in information management. These capabilities will support excellence and efficiency in our R&D programs by providing for optimal use of text, data, images, and sound in appropriate media. Employees will be proficient in the computer-related skills needed to realize fully the benefits from the Laboratory's information systems.

## **1. Information Technology**

### *Situation*

We provide a wide range of central services to support the digital collection, creation, dissemination, and archiving of R&D and business information. Service organizations also operate a Laboratory-wide spectrum of systems and services for software development and application, telecommunications, and computing. Strategic planning, funding, and coordinated management for the Laboratory's information infrastructure and systems are addressed collaboratively by policy and planning groups supported by review and implementation teams.

To ensure that our information management infrastructure evolves as required to support programmatic needs, we lead or collaborate in various national initiatives in information access, networking, and telecommunications, particularly through pilot projects that test the applicability of new information technologies to DOE-funded R&D. We maintain national network connections, such as ESnet (the DOE Energy Sciences Network), MREN (a high-speed test network in the Chicago metropolitan area, recently upgraded from 155 megabits per second to 622 megabits per second), and I-Wire (a statewide network test bed operating at 10 gigabits per second). Sophisticated network intrusion detection capabilities provide for identification and dynamic blocking of intruders and for detection of cyber security anomalies in network traffic. Each day, as many as 300,000 potential intruder alarms are scrutinized, and a terabyte of network traffic data is analyzed for cyber security anomalies.

### *Goals and Objectives*

The primary goal of information technology at Argonne is to maximize the ease and effectiveness with which information is acquired, created, communicated, stored, retrieved, and applied, both within the Laboratory and with our partners in government, academia, and the private sector. Our operations organizations have the following supporting objectives:

- Develop a comprehensive architecture for all aspects of information technology at the Laboratory.
- Streamline administrative operations by using rapid prototyping methods of application development.
- Develop and maintain an efficient, standards-based infrastructure for communications, computer networking, and information systems.
- Make the support organization for information technology more focused on solutions and more nimble.
- Seed collaboration technology to facilitate internal and external exchange of information.
- Maintain strong cyber security via both infrastructure and operational programs.
- Maintain strong core competencies in state-of-the-art and emerging information technologies that enable timely deployment of systems and services tailored to mission needs.
- Extend the currently available high-performance network to all Laboratory desktops.
- Evaluate emerging information technologies through aggressive use of demonstrations and pilot projects.

### *Strategies*

Our near-term strategies for information technology focus on the Laboratory's needs for (1) secure, high-performance telecommunications and networking infrastructure and (2) high-quality Laboratory-wide information systems and services.

Key strategies for achieving secure, high-performance, cost-effective network facilities include the following:

- Upgrade Laboratory network backbones and local connections to support seamless high-speed network access.
- Reengineer remote-access systems to allow secure use of Internet service providers.
- Ensure our interoperability with other DOE sites and commercial service providers through the continued use of test beds based on standards adopted at the Laboratory.
- Test and plan for an upgrade of the existing PBX (private branch exchange) system to an integrated voice-data-video network based on “Voice-over-IP” technology, which uses Internet protocol.

We operate a suite of central information systems in the areas of records, finance, personnel, procurement, facilities, scientific and technical information, environmental protection, and employee health and safety. Key strategies for achieving high-quality, cost-effective central information systems include the following:

- Pursue new initiatives that improve Laboratory-wide access to data supporting both R&D and operations.
- Simplify user access to operational and administrative information through expanded use of web interfaces.
- Build the information infrastructure needed to facilitate the migration of existing incompatible business applications to more open, integrated, web-based solutions.

## 2. Scientific and Technical Information

### *Situation*

Scientific and technical information (STI) is both an essential driver and the main product of our R&D. We manage our STI via an integrated suite of programmatic and support activities. Infrastructure that supports effective stewardship of STI throughout its life cycle includes virtual and physical library systems, publishing and

presentation services, and records management services.

Through digital, print, and staff resources, our research library provides efficient, structured access to the full range of global scientific and engineering information needed to undertake R&D. The Argonne Information Management (AIM) System is the key mechanism for delivering both internal and international library resources to researchers. Serving as a web portal to multidisciplinary information resources and services at Argonne and around the world, the AIM System averages about 21,000 user sessions per month. Over the past five years, customer usage of this system has increased 79%, and the average cost per use has dropped 30%.

Dissemination of results from our R&D is made more effective by centralized publishing and presentation support services at both major Argonne sites. These services encompass communications planning, writing, editing, the visual arts, and document production, with award-winning products in all conventional and digital media. The full text of each document published at the Laboratory or having an Argonne author is posted to web-based archives and made available to the global scientific community.

Our central records management services support the preservation of scientific and business information in accord with federal requirements. Services provided include technical assistance to records originators; a records inventory system; storage, retention, and disposal of older records; and Laboratory-wide records searches.

### *Goals and Objectives*

The goal of STI management at Argonne is to enhance the quality, productivity, and recognition of our R&D by enabling scientists and engineers to acquire and use relevant information rapidly and to communicate their findings effectively. Supporting objectives are (1) to provide high-performance digital systems and human services that give rapid, easy, continually improving access to STI and (2) to operate STI systems and services cost-effectively.

### Strategies

Key strategies for providing high-performance STI systems and services include the following:

- Influence the direction of electronic publishing to the benefit of Argonne and other national laboratories through collaboration with private-sector publishers, other research institutions, and federal agencies, taking advantage of national and international forums such as the John Wiley & Sons, Inc., Publishers Library Advisory Board and the INSPEC Library Advisory Council of the Institute of Electrical Engineers.
- Integrate industry-leading, standards-based, commercial hardware and software systems, as well as forefront creative practices, into the Laboratory's communications, library, and records management functions.
- Apply insights from internal customer feedback and external peer reviews to enhance the quality of Argonne's STI infrastructure and services. One example of external review is entry of publication and presentation products into professional peer competitions, which annually bring substantial numbers of awards to the Laboratory.
- Enhance the STI resources available on the desktops of our researchers through the AIM System. The system's growing virtual library includes electronic journals, scientific databases, reports, standards, specialized search and retrieval tools, and inventories of Argonne-authored publications and Argonne records. In 2004, 70% of the 1,157 journal titles to which the research library subscribes are available to staff electronically.
- Coordinate Argonne's research library resources and services with those of the University of Chicago.
- Increase the global public availability of Argonne-authored technical reports and conference papers via both a Laboratory Internet site and DOE-operated information dissemination systems.

Key strategies for achieving cost-effective STI systems and services include the following:

- Leverage capabilities developed to acquire, use, and communicate STI to improve management of text-based business information. Current examples are the management of office copier rental programs by central document production groups at both major Argonne sites; the integrated management of scientific and business records; and the inclusion of Laboratory manuals, business correspondence, the *Prime Contract*, and forms in the research library's AIM System.
- Operate support organizations at both major Argonne sites to provide the STI systems and services that are most efficient when their management is centralized.
- Match the scope and timeliness of institutional STI services to the needs of Argonne's R&D programs, through collaborative planning and budgeting by programmatic and operations staff and management.
- Purchase library collection materials through cost-saving consortial agreements, such as those negotiated by the DOE laboratories' library consortium; link Argonne staff to external library collections of special value, notably those of the University of Chicago and other major research libraries in Illinois. Actively inform Laboratory researchers about the usefulness of these resources.
- Apply the best practices of industry to achieve efficiency in all STI activities.

## F. Communications, Outreach, and Community Relations

### Situation

To conduct its R&D operations efficiently and effectively, Argonne must have the confidence and support of its stakeholders. Our major non-DOE stakeholders include Argonne employees, the research community, local and national news media, the trade press, the broad national public, members of the public living near our two sites, the educational community, and potential licensees and research partners in industry. Accordingly, we take special care to maintain close, positive relationships with all of these

groups and to foster a climate of mutual trust. This effort involves constant attention to two-way communications that are accurate, clear, timely, and credible. An active and growing outreach program seeks to inform our constituents about our work and to involve them constructively in our activities.

The major elements of our programs in communications, outreach, and community relations involve the following activities:

- *Employee Communications.* Argonne's weekly employee newsletter is read in its entirety or in part by more than 99% of employees. Employee communications are also well served by daily sitewide electronic mail broadcasts, a continually updated intranet, a telephone INFO-line, on-site technical and scientific seminars and conferences, colloquia featuring renowned speakers, and a variety of special employee events. A recently consolidated web site helps employees find the myriad support services provided at the Laboratory, including access to business and scientific computer systems.
- *The Research Community.* Ongoing communications with peers in the research community are conducted by scientific staff who publish more than 2,500 research papers and reports annually and who participate in scientific and technical conferences — often presenting papers or sponsoring events.
- *Media Relations.* Our external communications efforts mainly target the news media, which constitute our major avenue for informing the national and local public about both the long-term value of scientific research in general and the benefits of Argonne and DOE-funded research in particular.
- *Trade Press.* The trade press is an important vehicle for informing industrial researchers and executives about our research and facilities, which can help industry solve its research problems and can lead to other productive relationships, such as R&D partnerships.
- *Community Relations.* Our wide-ranging community relations programs reach all of our

major stakeholder groups. These programs include site tours, special events, speeches by staff to external audiences, and a vast array of Argonne-sponsored conferences and seminars.

Communications and outreach are also important aspects of other major Laboratory activities discussed elsewhere in this *Institutional Plan*, notably science education (see Section IV.A.10) and technology transfer (see Section IV.D and Supplement 2).

### *Goals and Strategies*

We continually seek opportunities to further strengthen our programs in communications, outreach, and community relations. Pursuit of the following important opportunities is under way or being planned:

- We are increasing our traditional outreach to the general science news media through efforts such as increased representation at press briefings and annual meetings of professional research societies.
- We are augmenting outreach to all key audiences with a new monthly electronic newsletter, *What's New at Argonne*, to which anyone may subscribe.
- We have supplemented our widely read weekly employee newsletter with a successful and popular daily electronic newsletter distributed to all Argonne-East employees.
- *Frontiers* (our annual magazine of research highlights) and *logos* (our periodical magazine of science news and feature stories) are being repositioned to focus more tightly on key Argonne audiences.
- We have begun to reorganize and redesign our public web presence to present a consistent Argonne brand that emphasizes our roles and contributions as a member of the University of Chicago and DOE communities.
- We have strengthened and rejuvenated our Speakers Bureau through an aggressive outreach program, to make potential audiences more aware of our speakers and the relevance of their topics and expertise to the interests of stakeholder groups.

- We are planning a series of community events to be held in lieu of a public open house, which is not possible in light of current national security concerns.
- We will continue to work closely with DOE-Chicago Operations and its Argonne Site Office to nurture a series of quarterly meetings with leaders from communities neighboring Argonne-East. This highly successful Community Leaders Round Table keeps our neighbors informed about our activities and expected impacts to the surrounding area, and it provides an informal forum for feedback.

For more than a half century, we have benefited from remarkably strong community support, positive news media relations, and strong management commitment to communications and outreach. The strategies outlined above are designed to build on those successes.

## G. Performance Management

### Situation

The performance-based *Prime Contract* under which the University of Chicago operates Argonne for DOE specifies objectives, performance measures, and incentives that foster outstanding performance by the Laboratory. Since FY 1996, our performance has been evaluated by DOE on the basis of previously negotiated measures and expectations, as specified in

Appendix B of the *Prime Contract*. (The term of the current contract extends through September 2004.) Argonne’s performance ratings have consistently been in the range of excellent to outstanding. (See Figure V.5.)

### Goals

Performance management begins with identification — by top Argonne management, the University of Chicago, and DOE — of high-level performance goals in three broad areas:

- *Science and Technology.* Argonne will deliver innovative, forefront science and technology aligned with DOE strategic goals and will conceive, design, construct, and operate world-class user facilities, all in a safe, environmentally sound, efficient manner.
- *Contractor Management.* The University of Chicago will provide leadership, guidance, and oversight that add value to the overall management of Argonne.
- *Operations.* Argonne will conduct all work and operate facilities cost-effectively and with distinction to achieve integration with and support of its mission in the areas of science, technology, energy, and environment, plus full protection of its workers, users of its facilities, the public, and the environment.

### Strategies

Performance measures are developed for Argonne with the following criteria in mind:

- Contributes directly to or enhances the Laboratory’s ability to accomplish its R&D mission.
- Drives performance by concentrating on desired outcomes.
- Compels the Laboratory to focus on systems performance, cost-effectiveness, and continuous improvement of functions and services essential to its mission.
- Allows for meaningful analysis of trends and rates of change.

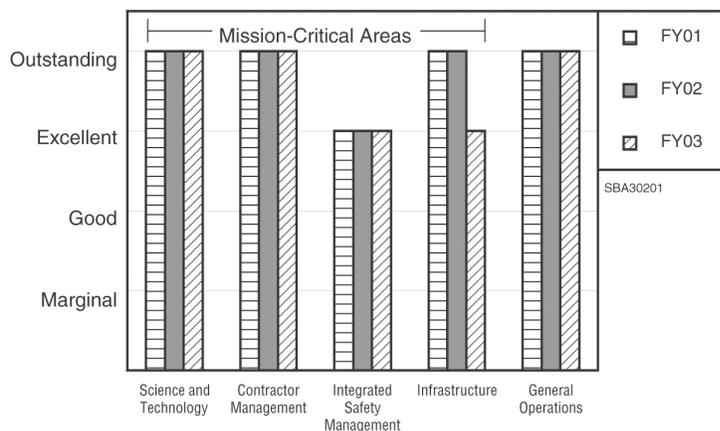


Figure V.5 Argonne Performance Ratings

- Adds commensurate value in the context of the Laboratory’s mission and its entire performance plan.

The Mission-Critical performance category considers functions that have direct and significant impact on the Laboratory’s ability to carry out its mission. Performance in these areas determines the annual fee received by the University of Chicago from DOE. In FY 2003 the Mission-Critical functions were science and technology, contractor management, ISM, and project and infrastructure management. Performance on project and infrastructure management was measured separately for Argonne-East and Argonne-West. Table V.3 gives examples of performance measures in the functional areas.

**Table V.3 Mission-Critical Functions — Examples of Performance Measures**

Functional Area	Measure
Science and Technology	Success in constructing and operating research facilities
Integrated Safety Management	Rate of days away from work
Project and Infrastructure Management	Actual costs and milestones compared to predetermined schedules
Leadership	Effective succession planning demonstrated for key personnel

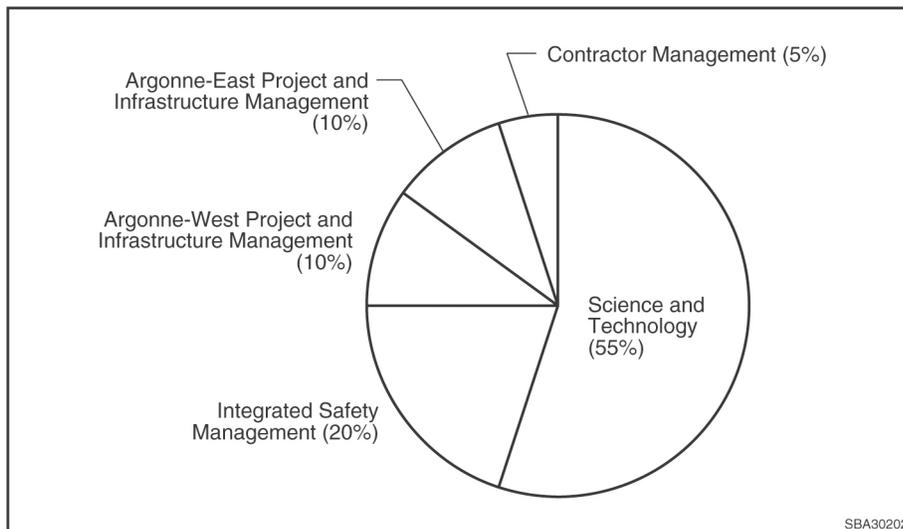
Figure V.6 indicates the weightings given the areas.

A number of operational activities not identified as critical are nevertheless included in Argonne’s performance management process. Performance in these general operations activities (see Table V.4) does not directly affect the University’s performance fee, but it does affect the size of the Laboratory’s annual employee bonus pool.

Working together, DOE, the University of Chicago, and Argonne have built strong momentum in continuously enhancing performance through ongoing feedback and improvement across the Laboratory. Ongoing improvement includes refinement of the measures used to drive performance, in order to better reflect desired outcomes and value added to the Laboratory’s research programs. As a general strategy, the university and the Laboratory are seeking to increase the use of peer review in the oversight and management of Laboratory operations.

**Table V.4 General Operations Functions**

Communications and trust	Legal management
Counterintelligence	Procurement
Cyber security	Property management
Finance	Safeguards and security
Human resources and diversity	Technology transfer
Information management	



**Figure V.6 Mission-Critical Functions by Contribution to Performance Fee (FY 2003)**



# VI. Resource Projections

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The resource projections in this chapter are considered a useful baseline for planning the desired near-term future of the Laboratory and for addressing important contingencies, particularly those associated with stringent federal budgets. The projections do not necessarily represent the outcome that the Laboratory considers most likely.

The resource projections extend through FY 2006, two years beyond the current year of FY 2004. (In earlier editions of this document, projections extended three additional years into the future.)

Because Argonne-West will be incorporated into the new Idaho National Laboratory during FY 2005, a separate Argonne-West funding summary table is provided for FY 2004 and FY 2005. This table is complemented by a separate Argonne-East funding summary table for FY 2004 through FY 2006. All other tables include Argonne-West funding through the full year of FY 2005, where appropriate, but exclude Argonne-West funding for FY 2006. For affected programs, particularly Nuclear Energy, Science and Technology, the result is an artificial funding decline in FY 2006.

The standard reporting date for information in the *Institutional Plan* is early spring of the year, so FY 2004 financial data in this chapter are midyear projections.

The projections show levels of activity at Laboratory, program, and subprogram levels. The resources required for Argonne's initiatives for years beyond FY 2004 generally are not included

in these resource projections. Funds received in FY 2003 and FY 2004 for initiatives are included in the funding levels shown for those years. Only funded and budgeted construction projects are included in the tables.

The figures for FY 2003 represent historical dollar values. The midyear projections for FY 2004 are in current dollars. Projections beyond FY 2004 incorporate annual cost escalation percentages that have been reviewed by DOE.

The resource projections are presented in 18 tables:

- Table VI.1 summarizes Laboratory total funding; Table VI.2 and Table VI.3 break out funding for Argonne-East and Argonne-West, respectively. Table VI.4 gives the total full-time-equivalent (FTE) personnel levels corresponding to the funding totals in Table VI.1.
- Tables VI.5 and VI.6, respectively, summarize total Laboratory funding and total personnel (FTE) levels for each DOE secretarial office.
- Tables VI.7-VI.18 give operating, capital equipment, and construction funding for each subprogram within specified DOE secretarial offices and for work supported by non-DOE organizations. Tables VI.7-VI.14 describe work funded directly by DOE, Table VI.15 considers work funded by DOE contractors, and Tables VI.16-VI.18 pertain to work funded by all other organizations.

**Table VI.1 Laboratory Funding Summary** (\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
DOE Funding	397.9	396.5	441.5	392.6
Work for Others (WFO) Program	96.4	100.4	104.0	102.8
Department of Homeland Security (DHS) Effort <sup>b</sup>	12.4	18.3	20.5	20.5
Additional Funding from Non-DOE Organizations	7.8	2.8	2.3	2.3
<b>Total Operating</b>	<b>514.5</b>	<b>518.0</b>	<b>568.3</b>	<b>518.2</b>
Capital Equipment <sup>c</sup>	17.7	27.1	30.7	39.1
Construction <sup>c,d</sup>	8.5	25.5	13.0	3.0
General Purpose Equipment	1.6	2.2	2.2	12.0
Accelerator Improvement Projects <sup>d</sup>	4.3	3.0	5.2	0.0
General Plant Projects <sup>d</sup>	8.2	14.3	6.8	0.0
Science Laboratories Infrastructure Program <sup>d</sup>	3.0	5.2	0.0	0.0
<b>Total Laboratory Funding</b>	<b>557.8</b>	<b>595.3</b>	<b>626.2</b>	<b>572.3</b>

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Includes direct funding from the Department of Homeland Security (DHS) and DHS work administered through the Work for Others program.

<sup>c</sup> Capital Equipment and Construction may include funding from sources other than DOE. The state of Illinois is projected to provide funds for (1) the Center for Nanoscale Materials building and (2) the Rare Isotope Accelerator Science Center building (see Table VI.18).

<sup>d</sup> Projections for Construction, Accelerator Improvement Projects, General Plant Projects, and Science Laboratories Infrastructure Program include only funded and budgeted projects. They do not include proposed projects and, unlike other funding categories, are not intended to represent a reasonable baseline for Laboratory planning in the later years of the planning horizon.

**Table VI.2 Laboratory Funding Summary — Argonne-East**  
(\$ in millions BA)

	FY 2004	FY 2005	FY 2006
DOE Funding	318.0	337.9	392.6
Work for Others (WFO) Program	98.8	103.9	102.8
Department of Homeland Security (DHS) Effort <sup>a</sup>	18.3	20.5	20.5
Additional Funding from Non-DOE Organizations	2.8	2.3	2.3
<b>Total Operating</b>	<b>437.9</b>	<b>464.6</b>	<b>518.2</b>
Capital Equipment <sup>b</sup>	26.2	30.3	39.1
Construction <sup>b,c</sup>	25.5	13.0	3.0
General Purpose Equipment	2.2	2.2	12.0
Accelerator Improvement Projects <sup>c</sup>	3.0	5.2	0.0
General Plant Projects <sup>c</sup>	5.5	5.0	0.0
Science Laboratories Infrastructure Program <sup>c</sup>	5.2	0.0	0.0
<b>Total Laboratory Funding</b>	<b>505.5</b>	<b>520.3</b>	<b>572.3</b>

<sup>a</sup> Includes direct funding from the Department of Homeland Security (DHS) and DHS work administered through the Work for Others program.

<sup>b</sup> Capital Equipment and Construction may include funding from sources other than DOE. The state of Illinois is projected to provide funds for (1) the Center for Nanoscale Materials building and (2) the Rare Isotope Accelerator Science Center building (see Table VI.16).

<sup>c</sup> Projections for Construction, Accelerator Improvement Projects, General Plant Projects, and Science Laboratories Infrastructure Program include only funded and budgeted projects. They do not include proposed projects and, unlike other funding categories, are not intended to represent a reasonable baseline for Laboratory planning in the later years of the planning horizon.

**Table VI.3 Laboratory Funding Summary — Argonne-West**  
(\$ in millions BA)

	FY 2004	FY 2005
DOE Funding	78.5	103.6
Work for Others (WFO) Program	1.6	0.1
Department of Homeland Security (DHS) Effort <sup>a</sup>	0.0	0.0
Additional Funding from Non-DOE Organizations	0.0	0.0
<b>Total Operating</b>	<b>80.1</b>	<b>103.7</b>
Capital Equipment <sup>b</sup>	0.9	0.4
Construction <sup>b,c</sup>	0.0	0.0
General Purpose Equipment	0.0	0.0
Accelerator Improvement Projects <sup>c</sup>	0.0	0.0
General Plant Projects <sup>c</sup>	8.8	1.8
Science Laboratories Infrastructure Program <sup>c</sup>	0.0	0.0
<b>Total Laboratory Funding</b>	<b>89.8</b>	<b>105.9</b>

<sup>a</sup> Includes direct funding from the Department of Homeland Security (DHS) and DHS work administered through the Work for Others program.

<sup>b</sup> Capital Equipment and Construction may include funding from sources other than DOE. The state of Illinois is projected to provide funds for (1) the Center for Nanoscale Materials building and (2) the Rare Isotope Accelerator Science Center building (see Table VI.16).

<sup>c</sup> Projections for Construction, Accelerator Improvement Projects, General Plant Projects, and Science Laboratories Infrastructure Program include only funded and budgeted projects. They do not include proposed projects and, unlike other funding categories, are not intended to represent a reasonable baseline for Laboratory planning in the later years of the planning horizon.

**Table VI.4 Laboratory Personnel Summary (in FTE)**

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
Direct Personnel				
DOE Effort	1701.4	1733.0	1819.9	1449.4
Work for Others (WFO) Program	289.6	313.7	330.1	312.2
Department of Homeland Security (DHS) Effort <sup>b</sup>	16.0	12.2	13.1	12.6
Additional Funding from Non-DOE Organizations <sup>c</sup>	4.6	1.3	1.9	1.8
Subtotal	2011.6	2060.2	2165.0	1776.0
Other Direct <sup>d</sup>	558.1	522.4	443.2	354.6
Total Direct Personnel	2569.7	2582.6	2608.2	2130.6
Indirect Personnel	1295.8	1158.0	1158.0	957.5
Total Personnel	3865.5	3740.6	3766.2	3088.1

<sup>a</sup> The personnel projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Full-time equivalents reflect direct funding from the Department of Homeland Security (DHS) and DHS work administered through the Work for Others program.

<sup>c</sup> Includes FTEs associated with services provided to Advanced Photon Source users and work for partners in cooperative R&D agreements.

<sup>d</sup> The "other direct" personnel category includes FTEs for general Laboratory services, program management and administration, staff temporary assignments, and Laboratory Directed Research and Development.

**Table VI.5 Funding by Assistant Secretarial Office (\$ in millions BA)**

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>DOE WORK</b>				
<b>Table VI.7 — Science</b>				
Operating	207.5	215.4	225.2	264.8
Capital Equipment	16.9	25.7	28.0	36.3
General Purpose Equipment	1.6	2.2	2.2	12.0
Accelerator Improvement Projects <sup>b</sup>	4.3	3.0	5.2	0.0
General Plant Projects <sup>b</sup>	5.6	5.5	5.0	0.0
Subtotal	235.9	251.8	265.6	313.1
Science Laboratories Infrastructure Program <sup>b</sup>	3.0	5.2	0.0	0.0
Total Science	238.9	257.0	265.6	313.1
<b>Table VI.8 — Nuclear Energy, Science and Technology</b>				
Operating	82.0	83.8	86.3	19.9
Capital Equipment	0.6	0.9	0.4	0.0
General Plant Projects <sup>b</sup>	2.6	8.8	1.8	0.0
Total	85.2	93.5	88.5	19.9
<b>Table VI.9 — Energy Efficiency and Renewable Energy</b>				
Operating	37.1	41.1	45.3	45.8
Capital Equipment	0.2	0.5	1.7	2.3
Total	37.3	41.6	47.0	48.1
<b>Table VI.10 — Fossil Energy</b>				
Operating	5.1	5.7	6.0	5.4
<b>Table VI.11 — Environmental Management</b>				
Operating	6.3	3.1	13.2	2.6
<b>Table VI.12 — National Nuclear Security Administration</b>				
Operating	24.4	22.9	37.7	18.4
Capital Equipment	0.0	0.0	0.1	0.0
Total	24.4	22.9	37.8	18.4
<b>Table VI.13 — Security and Emergency Operations</b>				
Operating	0.8	1.0	1.1	1.1
<b>Table VI.14 — Other DOE Programs<sup>c</sup></b>				
Operating	6.2	4.9	8.4	8.6

Table VI.5 Funding by Assistant Secretarial Office (Cont.)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Table VI.15 — Work for Other DOE Contractors</b>				
Operating	28.5	18.6	18.3	26.0
<b>TOTAL WORK FOR DOE PROGRAMS</b>				
Operating	397.9	396.5	441.5	392.6
Capital Equipment	17.7	27.1	30.7	39.1
General Purpose Equipment	1.6	2.2	2.2	12.0
Accelerator Improvement Projects <sup>b</sup>	4.3	3.0	5.2	0.0
General Plant Projects <sup>b</sup>	8.2	14.3	6.8	0.0
Subtotal	429.7	443.1	486.4	443.7
Science Laboratories Infrastructure Program <sup>b</sup>	3.0	5.2	0.0	0.0
Total	432.7	448.3	486.4	443.7
<b>Table VI.16 — Work for Others (WFO) Program</b>				
Operating	96.4	100.4	104.0	102.8
<b>Table VI.17 — Department of Homeland Security Effort</b>				
Operating	12.4	18.3	20.5	20.5
<b>Table VI.18 — Additional Funding from Non-DOE Organizations</b>				
Operating	7.8	2.8	2.3	2.3
Construction	8.5	25.5	13.0	3.0
Total	16.3	28.3	15.3	5.3
<b>TOTAL OPERATING FUNDING</b>	514.5	518.0	568.3	518.2
<b>TOTAL CAPITAL EQUIPMENT</b>	17.7	27.1	30.7	39.1
<b>TOTAL CONSTRUCTION<sup>b</sup></b>	8.5	25.5	13.0	3.0
<b>TOTAL GENERAL PURPOSE EQUIPMENT</b>	1.6	2.2	2.2	12.0
<b>TOTAL ACCELERATOR IMPROVEMENT PROJECTS<sup>b</sup></b>	4.3	3.0	5.2	0.0
<b>TOTAL GENERAL PLANT PROJECTS<sup>b</sup></b>	8.2	14.3	6.8	0.0
<b>TOTAL SCIENCE LABORATORIES INFRASTRUCTURE PROGRAM<sup>b</sup></b>	3.0	5.2	0.0	0.0

Table VI.5 Funding by Assistant Secretarial Office (Cont.)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>GRAND TOTAL LABORATORY FUNDING</b>	557.8	595.3	626.2	572.3

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Projections for Construction, Accelerator Improvement Projects, General Plant Projects, and Science Laboratories Infrastructure Program include only funded and budgeted projects. They do not include proposed projects and, unlike other funding categories, are not intended to represent a reasonable baseline for Laboratory planning in the later years of the planning horizon.

<sup>c</sup> Other DOE programs include B&R codes WN-05, HC, HD, PE, CN, TD, and DF. (See Table VI.14.)

Table VI.6 Personnel by Assistant Secretarial Office (in FTE)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>DOE WORK</b>				
<b>Science</b>	921.4	941.8	971.5	1028.8
<b>Nuclear Energy, Science and Technology</b>	387.5	383.2	365.6	67.1
<b>Energy Efficiency and Renewable Energy</b>	134.8	148.5	154.7	153.8
<b>Fossil Energy</b>	21.6	27.9	24.3	22.0
<b>Environmental Management</b>	23.3	14.8	47.9	7.6
<b>National Nuclear Security Administration</b>	79.4	92.1	121.6	52.6
<b>Security and Emergency Operations</b>	2.4	2.9	2.9	2.6
<b>Other DOE Programs<sup>b</sup></b>	26.9	19.2	28.8	26.7
<b>Work for Other DOE Contractors</b>	104.1	102.6	102.6	88.2
<b>Work for Others (WFO) Program</b>	289.6	313.7	330.1	312.2
<b>Department of Homeland Security<sup>c</sup></b>	16.0	12.2	13.1	12.6
<b>Additional Funding from Non-DOE Organizations<sup>d</sup></b>	4.6	1.3	1.9	1.8
<b>SUBTOTAL</b>	2011.6	2060.2	2165.0	1776.0
<b>Other Direct<sup>e</sup></b>	558.1	522.4	443.2	354.6
<b>Total Direct Personnel</b>	2569.7	2582.6	2608.2	2130.6
<b>Indirect Personnel</b>	1295.8	1158.0	1158.0	957.5
<b>Total Personnel</b>	3865.5	3740.6	3766.2	3088.1

<sup>a</sup> The personnel projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Includes B&R codes WN-05, HC, HD, PE, CN, TD, and DF. (See Table VI.14.)

<sup>c</sup> Full-time equivalents reflect direct funding from the Department of Homeland Security (DHS) and DHS work administered through the Work for Others program.

<sup>d</sup> Includes FTEs associated with services provided to Advanced Photon Source users and work for partners in cooperative R&D agreements.

<sup>e</sup> The "other direct" personnel category includes FTEs for general Laboratory services, program management and administration, staff temporary assignments, and Laboratory Directed Research and Development.

**Table VI.7 Science: Funding by Subprogram** (\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Fusion Energy Sciences (AT)</b>				
Operating	1.3	0.7	1.2	1.5
Capital Equipment	0.0	0.3	0.0	0.0
Total	1.3	1.0	1.2	1.5
<b>Safeguards and Security — Science (FS-10)</b>				
Operating	7.3	7.3	9.4	10.1
<b>Proton Accelerator-Based Physics (KA-11)</b>				
Operating	4.5	6.2	6.2	8.2
Capital Equipment	1.4	1.6	1.4	0.9
Total	5.9	7.8	7.6	9.1
<b>Theoretical Physics (KA-14)</b>				
Operating	1.5	1.5	1.5	1.6
<b>Advanced Technology R&amp;D (KA-15)</b>				
Operating	2.1	1.3	1.4	1.5
Capital Equipment	0.1	0.1	0.1	0.2
Total	2.2	1.4	1.5	1.7
<b>Total High Energy Physics (KA)</b>				
Operating	8.1	9.0	9.1	11.3
Capital Equipment	1.5	1.7	1.5	1.1
Total	9.6	10.7	10.6	12.4
<b>Nuclear Physics (KB)</b>				
Operating	18.5	18.1	19.2	25.3
Capital Equipment	1.9	1.2	1.4	2.8
Accelerator Improvement Projects <sup>b</sup>	0.4	0.4	1.2	0.0
Total	20.8	19.7	21.8	28.1
<b>Materials Sciences (KC-02)</b>				
Operating	35.8	36.8	37.7	39.1
Capital Equipment	5.5	15.6	17.1	20.2
Total	41.3	52.4	54.8	59.3
<b>Advanced Photon Source (KC-02)</b>				
Operating	81.6	86.8	87.4	105.0
Capital Equipment	5.4	5.0	6.0	8.8
Accelerator Improvement Projects <sup>b</sup>	3.9	2.6	4.0	0.0
Total	90.9	94.4	97.4	113.8

Table VI.7 Science: Funding by Subprogram (Cont.)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Total Materials Sciences (KC-02)</b>				
Operating	117.4	123.6	125.1	144.1
Capital Equipment	10.9	20.6	23.1	29.0
Accelerator Improvement Projects <sup>b</sup>	3.9	2.6	4.0	0.0
Total	132.2	146.8	152.2	173.1
<b>Chemical Sciences (KC-03)</b>				
Operating	15.1	14.9	14.9	18.7
Capital Equipment	2.2	1.7	1.7	2.2
General Purpose Equipment	1.6	2.2	2.2	12.0
General Plant Projects <sup>b</sup>	5.6	5.5	5.0	0.0
Total	24.5	24.3	23.8	32.9
<b>Total Basic Energy Sciences (KC-02, KC-03)</b>				
Operating	132.5	138.5	140.0	162.8
Capital Equipment	13.1	22.3	24.8	31.2
General Purpose Equipment	1.6	2.2	2.2	12.0
Accelerator Improvement Projects <sup>b</sup>	3.9	2.6	4.0	0.0
General Plant Projects <sup>b</sup>	5.6	5.5	5.0	0.0
Total	156.7	171.1	176.0	206.0
<b>Excess Facilities Disposition Program (KG)</b>				
Operating	1.1	1.8	2.1	2.1
<b>Mathematical, Information, and Computational Sciences (KJ-01)</b>				
Operating	12.4	11.5	14.9	16.1
Capital Equipment	0.0	0.0	0.0	0.8
Total	12.4	11.5	14.9	16.9
<b>Total Computational and Technology Research (KJ)</b>				
Operating	12.4	11.5	14.9	16.1
Capital Equipment	0.0	0.0	0.0	0.8
Total	12.4	11.5	14.9	16.9
<b>Workforce Development for Teachers and Scientists (KL)</b>				
Operating	1.6	2.1	2.6	2.6
<b>Life Sciences (KP-11)</b>				
Operating	4.6	5.2	5.8	6.0
Capital Equipment	0.2	0.2	0.3	0.3
Total	4.8	5.4	6.1	6.3

Table VI.7 Science: Funding by Subprogram (Cont.)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Environmental Processes (KP-12)</b>				
Operating	18.4	19.1	19.1	24.9
Capital Equipment	0.0	0.0	0.0	0.1
Total	18.4	19.1	19.1	25.0
<b>Environmental Remediation (KP-13)</b>				
Operating	1.5	1.7	1.4	1.7
<b>Medical Applications and Measurement Science (KP-14)</b>				
Operating	0.2	0.4	0.4	0.4
Capital Equipment	0.2	0.0	0.0	0.0
Total	0.4	0.4	0.4	0.4
<b>Total Biological and Environmental Research (KP)</b>				
Operating	24.7	26.4	26.7	33.0
Capital Equipment	0.4	0.2	0.3	0.4
Total	25.1	26.6	27.0	33.4
<b>Total Science</b>				
Operating	207.5	215.4	225.2	264.8
Capital Equipment	16.9	25.7	28.0	36.3
General Purpose Equipment	1.6	2.2	2.2	12.0
Accelerator Improvement Projects <sup>b</sup>	4.3	3.0	5.2	0.0
General Plant Projects <sup>b</sup>	5.6	5.5	5.0	0.0
Subtotal	235.9	251.8	265.6	313.1
Science Laboratories Infrastructure Program <sup>b</sup>	3.0	5.2	0.0	0.0
Total Science	238.9	257.0	265.6	313.1

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Projections for Construction, Accelerator Improvement Projects, General Plant Projects, and Science Laboratories Infrastructure Program include only funded and budgeted projects. They do not include proposed projects and, unlike other funding categories, are not intended to represent a reasonable baseline for Laboratory planning in the later years of the planning horizon.

**Table VI.8 Nuclear Energy, Science and Technology: Funding by Subprogram (\$ in millions BA)**

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Nuclear Energy Research and Development (AF)</b>				
Operating	75.4	76.3	77.8	19.9
Capital Equipment	0.6	0.9	0.4	0.0
General Plant Projects <sup>b</sup>	1.6	8.6	1.8	0.0
Total	77.6	85.8	80.0	19.9
<b>Safeguards and Security — Nuclear Energy (FS-55)</b>				
Operating	6.6	7.5	8.5	0.0
General Plant Projects <sup>b</sup>	1.0	0.2	0.0	0.0
Total	7.6	7.7	8.5	0.0
<b>Total Nuclear Energy, Science and Technology</b>				
Operating	82.0	83.8	86.3	19.9
Capital Equipment	0.6	0.9	0.4	0.0
General Plant Projects <sup>b</sup>	2.6	8.8	1.8	0.0
Total	85.2	93.5	88.5	19.9

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Projections for Construction, Accelerator Improvement Projects, General Plant Projects, and Science Laboratories Infrastructure Program include only funded and budgeted projects. They do not include proposed projects and, unlike other funding categories, are not intended to represent a reasonable baseline for Laboratory planning in the later years of the planning horizon.

**Table VI.9 Energy Efficiency and Renewable Energy: Funding by Subprogram**  
(\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Biomass Energy Technologies (BM)</b>				
Operating	0.3	0.1	0.1	0.1
<b>Solar and Renewable Resource Technologies (EB)</b>				
Operating	1.1	1.1	1.3	1.4
<b>Industry Sector (ED)</b>				
Operating	2.7	4.3	3.4	2.7
Capital Equipment	0.2	0.0	0.0	0.0
Total	2.9	4.3	3.4	2.7
<b>Policy and Management (EH)</b>				
Operating	1.0	0.9	1.2	1.2
<b>Distributed Energy Resources (EO-01)</b>				
Operating	1.5	2.4	3.1	3.1
<b>Fuel Cell Technologies (HI)</b>				
Operating	9.1	8.9	9.3	9.8
Capital Equipment	0.0	0.3	0.4	0.5
Total	9.1	9.2	9.7	10.3
<b>Vehicle Technology (VT)</b>				
Operating	20.8	23.2	26.4	27.0
Capital Equipment	0.0	0.2	1.3	1.8
Total	20.8	23.4	27.7	28.8
<b>Weatherization and Intergovernmental Programs (WI)</b>				
Operating	0.6	0.2	0.5	0.5
<b>Total Energy Efficiency and Renewable Energy</b>				
Operating	37.1	41.1	45.3	45.8
Capital Equipment	0.2	0.5	1.7	2.3
Total	37.3	41.6	47.0	48.1

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

**Table VI.10 Fossil Energy: Funding by Subprogram** (\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Coal (AA)</b>				
Operating	4.0	4.0	4.7	4.2
<b>Gas (AB)</b>				
Operating	0.5	0.6	0.4	0.2
<b>Petroleum (AC)</b>				
Operating	0.6	0.9	0.7	0.7
<b>Gas and Electricity (AU)</b>				
Operating	0.0	0.2	0.2	0.3
<b>Total Fossil Energy</b>				
Operating	5.1	5.7	6.0	5.4

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

**Table VI.11 Environmental Management: Funding by Subprogram** (\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Environmental Restoration and Waste Management — Defense (EW)</b>				
Operating	0.2	0.0	0.0	0.0
<b>Environmental Management — Defense (EY)</b>				
Operating	1.8	1.3	1.7	1.5
<b>Environmental Management — Non-Defense (EZ)</b>				
Operating	4.3	1.8	11.5	1.1
<b>Total Environmental Management</b>				
Operating	6.3	3.1	13.2	2.6

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

**Table VI.12 National Nuclear Security Administration: Funding by Subprogram**  
(\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Weapons Activities (DP)</b>				
Operating	1.8	2.8	2.4	2.4
Capital Equipment	0.0	0.0	0.1	0.0
Total	1.8	2.8	2.5	2.4
<b>Defense Nuclear Nonproliferation (NN)<sup>b</sup></b>				
Operating	22.6	20.0	35.2	15.9
<b>Program Direction — National Nuclear Security Administration (PS)</b>				
Operating	0.0	0.1	0.1	0.1
<b>Total National Nuclear Security Administration</b>				
Operating	24.4	22.9	37.7	18.4
Capital Equipment	0.0	0.0	0.1	0.0
Total	24.4	22.9	37.8	18.4

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> For FY 2003, funding for B&R code NN-2004 is excluded here and included instead in Department of Homeland Security effort (Table VI.17).

**Table VI.13 Security and Emergency Operations: Funding by Subprogram**  
(\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Nuclear Safeguards and Security (GD)</b>				
Operating	0.8	0.9	1.0	1.0
<b>Office of Security (OS)</b>				
Operating	0.0	0.1	0.1	0.1
<b>Total Security and Emergency Operations</b>				
Operating	0.8	1.0	1.1	1.1

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

**Table VI.14 Other DOE Programs: Operating Funding by Assistant Secretary**  
(\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Management, Budget, and Evaluation (WN-05)<sup>b</sup></b>	1.1	1.1	1.1	1.1
<b>Environment, Safety, and Health (HC, HD)</b>	0.5	0.5	0.5	0.5
<b>Policy and International Affairs (PE)</b>	0.0	0.1	0.1	0.1
<b>Counterintelligence (CN)</b>	1.1	1.2	1.4	1.4
<b>Electric Transmission and Distribution (TD)</b>	3.3	1.1	4.6	5.0
<b>Civilian Radioactive Waste Management (DF)</b>	0.2	0.9	0.7	0.5
<b>Total Other DOE Programs</b>	6.2	4.9	8.4	8.6

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Recovery of safeguards and security costs associated with work for sponsors other than DOE.

**Table VI.15 Work for Other DOE Contractors** (\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
Operating	28.5	18.6	18.3	26.0

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

Table VI.16 Work for Others (WFO) Program: Operating Funding (\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>NUCLEAR REGULATORY COMMISSION</b>	12.0	12.0	10.5	10.5
<b>DEPARTMENT OF DEFENSE</b>				
U.S. Air Force	1.7	2.5	2.7	2.7
The Joint Staff	2.7	2.8	2.7	2.7
U.S. Army	12.0	12.5	13.6	13.6
U.S. Navy	2.2	4.0	4.6	4.6
Defense Threat Reduction Agency	0.6	3.5	3.8	3.8
Defense Advanced Research Projects Agency	1.3	2.4	2.7	2.7
Other Defense	0.2	3.5	3.5	3.5
<b>Total Department of Defense</b>	<b>20.7</b>	<b>31.2</b>	<b>33.6</b>	<b>33.6</b>
<b>OTHER FEDERAL AGENCIES</b>				
Environmental Protection Agency	2.2	2.1	2.3	2.3
Department of State (International Atomic Energy Agency)	3.2	3.4	3.8	3.8
Department of Health and Human Services <sup>b</sup>	7.1	4.4	4.9	4.9
Department of Agriculture	7.7	7.5	8.2	8.2
National Aeronautics and Space Administration	1.9	1.7	1.8	1.8
Department of the Interior	1.7	1.5	1.6	1.6
Other Agencies	0.1	1.2	1.7	1.7
<b>Total Other Federal Agencies</b>	<b>23.9</b>	<b>21.8</b>	<b>24.3</b>	<b>24.3</b>
<b>NONFEDERAL ORGANIZATIONS</b>				
Private Firms	16.6	12.9	8.1	7.9
Universities	5.2	5.2	6.4	6.4
University of Chicago Grants <sup>b</sup>	14.1	12.5	17.4	16.6
State and Local Governments	1.5	2.7	2.8	2.3

**Table VI.16 Work for Others (WFO) Program: Operating Funding (Cont.)**

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>International Organizations and Foreign Countries</b>	2.4	2.1	0.9	1.2
<b>Total Nonfederal Organizations</b>	39.8	35.4	35.6	34.4
<b>TOTAL WORK FOR OTHERS (WFO) PROGRAM</b>	96.4	100.4	104.0	102.8

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Grants that are funded by the National Institutes of Health are reported as University of Chicago Grants.

**Table VI.17 Department of Homeland Security Effort (\$ in millions BA)**

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>a</sup>
<b>Department of Homeland Security<sup>b</sup></b>				
Operating	12.4	18.3	20.5	20.5

<sup>a</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>b</sup> Reflects direct funding from the Department of Homeland Security (DHS) and DHS work administered through the Work for Others program.

**Table VI.18 Additional Funding from Non-DOE Organizations<sup>a</sup>**  
(\$ in millions BA)

	FY 2003	FY 2004	FY 2005	FY 2006 <sup>b</sup>
<b>CRADA Partners</b>				
Operating	0.4	0.2	0.3	0.3
<b>Services to APS Users</b>				
Operating	7.4	2.6	2.0	2.0
<b>Illinois State Government Grants<sup>c</sup></b>				
Operating	0.0	0.0	0.0	0.0
Construction	8.5	25.5	13.0	3.0
Total	8.5	25.5	13.0	3.0
<b>Total Additional Funding from Non-DOE Organizations</b>				
Operating	7.8	2.8	2.3	2.3
Construction	8.5	25.5	13.0	3.0
Total	16.3	28.3	15.3	5.3

<sup>a</sup> Certain work performed by Argonne for non-DOE sponsors is neither administered under the Laboratory's Work for Others program nor sponsored by the Department of Homeland Security and so is considered separately in this table. Included here are (1) funds received from cooperative R&D agreement (CRADA) partners, (2) funds received from collaborative access teams at the APS for services performed, and (3) grants from the state of Illinois.

<sup>b</sup> The funding projection for FY 2006 includes Argonne-East only.

<sup>c</sup> Funding from the state of Illinois for (1) the Center for Nanoscale Materials building and (2) the Rare Isotope Accelerator Science Center building.

# Supplement 1: Work for Sponsors other than DOE

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Our work for non-DOE sponsors supports accomplishment of our mission (see Chapter II) and development of our initiatives (see Chapter III). This “work for others” (WFO) allows our unique facilities and capabilities to be applied to national security needs and other national R&D priorities.

Our WFO strengthens resources available for DOE missions and programs and promotes development of specific energy and environmental technologies. Furthermore, this WFO enhances our research capabilities, helps support the infrastructure at the Laboratory, and ultimately increases opportunities to transfer our technologies to productive applications in the private sector. Argonne does not undertake work for non-DOE sponsors if that work can be performed satisfactorily by private organizations.

In the area of national security, we perform a wide range of work funded by federal organizations other than DOE, including the new Department of Homeland Security (DHS). In the area of national security we also provide R&D, technical support, and training for the Departments of Defense and Transportation, as well as for the Nuclear Regulatory Commission.

Our other major non-DOE sponsors include the Department of Health and Human Services, the Environmental Protection Agency, the Department of State, the Department of Agriculture, the National Science Foundation, the National Aeronautics and Space Administration, the Department of Commerce, the Department of the Interior, the Electric Power Research Institute (EPRI), private organizations, universities, and state and local governments. (See Chapter VI for program funding.)

The concluding section of this Supplement 1 describes Argonne work sponsored directly by DHS. Generally speaking, this work is performed on the same basis as work for DOE and is not subject to the restrictions applied to work for most non-DOE sponsors.

## A. Nuclear Regulatory Commission

We conduct research for the Nuclear Regulatory Commission (NRC) under a legislatively mandated memorandum of understanding between DOE and the NRC. Most of our work for the NRC has for many years involved supporting the Office of Nuclear Regulatory Research in its development of rules regarding plant safety and the condition of physical components. The largest efforts have addressed materials issues, steam generator tubing degradation, high-burnup fuel, and severe-accident behavior. Recently Argonne performed studies to (1) enhance environmental pathway models for analyzing the transport of residual radioactive contaminants and (2) develop parameters suitable for implementing NRC rules designed to assure public health and safety at nuclear facilities during the termination of licensed operations. We are now preparing portions of supplemental environmental impact statements for the renewal of reactor operating licenses. In addition, Argonne provides technical assistance to the Office of Nuclear Reactor Regulation and to the Office of Nuclear Materials Safety and Safeguards.

Both the research and the technical assistance for the NRC take advantage of the Laboratory’s hot cells and its special capabilities in nuclear reactor technology, technical evaluation, systems analysis, materials science, computer code development, environmental risk modeling, and assessment of environmental and health impacts. Argonne’s work helps to ensure that U.S. nuclear power plants will continue their safe, efficient production of electricity without emission of combustion products or greenhouse gases.

### 1. Office of Nuclear Regulatory Research

Our materials research focuses on the degradation of structural materials in the harsh environments of light-water reactors, including the effects of water chemistry and neutron

irradiation. These studies include measurements of (1) growth rates of stress corrosion cracks in irradiated and nonirradiated materials and (2) the fatigue life of stainless and ferritic steels used in the reactor core, piping, and pressure vessel. Results from these studies are used by the NRC to ensure the structural integrity of plants as they age. Currently, we are examining portions of a leaking nozzle and a degraded pressure vessel head from the Davis Besse plant.

A comprehensive study of degradation in the steam generator tubing of nuclear power plants is under way. Critical areas being addressed include (1) evaluation of techniques used for in-service inspection of steam generator tubes and recommendations for improving the reliability and accuracy of those inspections, (2) validation and improvement of correlations and models for predicting degradation in aging tubes during operations, and (3) investigation of the potential for environmental degradation of Alloy 690, which has been used in most replacement generators in the United States.

Argonne is investigating the behavior of high-burnup nuclear fuels for the NRC. To reduce operating costs and minimize the accumulation of spent fuel, nuclear utilities are striving to increase the burnup of their nuclear fuels. However, at high burnups, fuel pellets and cladding are potentially less resistant to damage under some conditions. These considerations may necessitate modification of (1) fuel rod damage criteria used in NRC regulations and (2) materials properties assumed in safety analyses. Furthermore, new alloys and fabrication procedures designed to counter burnup effects may also affect regulatory criteria and safety analyses. To help address these issues, Argonne is investigating the behavior of high-burnup fuel under accident conditions where coolant is lost, as well as which mechanical properties of high-burnup cladding must be determined for licensing and safety analyses. The Laboratory is also investigating the way high burnup might affect cladding and the behavior of spent fuel during long-term dry storage, a strategy now being employed at the sites of many nuclear power plants.

The NRC continues to use Argonne's broad expertise in severe-accident phenomena. The NRC was a partner in the recently completed Melt

Attack and Coolability Experiment (MACE) program organized by EPRI. The Laboratory's contributions to this program are described in Section S1.E.1. The NRC will continue to benefit from Argonne's expertise in this area through our participation in the Melt Coolability and Concrete Interaction program, a follow-on to MACE sponsored by the Organization for Economic Cooperation and Development (see Section S1.E.5).

The NRC license termination rule assures public health and safety at nuclear facilities during the termination of licensed operations. To support the development of implementation guidance for this rule and an associated standard review plan, the NRC is using the Argonne software RESidual RADioactivity (RESRAD), previously expanded under NRC sponsorship. The expanded program will specifically address the cleanup of contaminated sites and buildings during the decontamination and decommissioning (D&D) of facilities. The RESRAD software was originally developed for DOE to help analyze environmental remediation at DOE sites. The NRC-sponsored work extended the existing models to include probabilistic dose analyses, thereby allowing NRC licensees to demonstrate compliance with the license termination rule and supporting NRC evaluation of the licensees' applications for facility termination.

We are initiating work on an alternative siting rule for the NRC to use in evaluating new reactor sites. The NRC will use this rule to evaluate alternatives in applications it receives for an early site permit and a combined construction-operation license.

## 2. Office of Nuclear Reactor Regulation

Argonne assists the NRC Office of Nuclear Reactor Regulation in a variety of areas related to aging and the performance of materials, components, structures, and systems in nuclear power plants. This work helps assure that safety is maintained as plant components age.

Argonne provides technical support to the NRC in the review of license renewal applications in areas including fatigue of metal components, thermal fatigue of cast austenitic stainless steels,

irradiation-assisted stress corrosion cracking, and irradiation-induced void swelling.

We participate on interlaboratory teams preparing supplemental environmental impact statements related to the renewal of nuclear plant operating licenses. These analyses have covered issues of land use, ecology, and air quality that are related to continued power plant operations.

The Laboratory is reviewing aging effects and their management for nuclear plant systems, structures, and components that must meet license renewal rules. Previous work contributed to the development of a report and an associated standard review plan that serve as guidance documents for NRC reviews of license renewal applications. We are currently updating and revising this guidance. Argonne also provides other kinds of technical support to the Office of Nuclear Reactor Regulation.

### **3. Office of Nuclear Materials Safety and Safeguards**

For the Office of Nuclear Materials Safety and Safeguards, we are modeling environmental and health effects from uranium recovery operations to help the NRC (1) deal with changes in regulatory requirements and (2) consider revisions of existing licenses and applications for new licenses for uranium mining and processing. Enhancements of the current model will take into account *in situ* uranium leaching technology and associated processing. A key issue is the transport of uranium and decay product radionuclides (including radon gas), as well as the associated environmental and health impacts. At the same time, we are developing an Internet-based communication mechanism to facilitate distribution of the software code for the model and the NRC's interaction with prospective licensees. In other work, we are helping to prepare an environmental impact statement for construction and operation of a mixed-oxide fuel fabrication facility to be built at the DOE Savannah River Site. The facility will convert surplus weapons-grade plutonium into mixed-oxide fuel suitable for irradiation in light-water reactors.

## **B. Department of Defense**

Argonne conducts research for several organizations within the Department of Defense (DOD).

### **1. U.S. Air Force**

The U.S. Air Force sponsors several programs at Argonne. Our experience and expertise in conducting environmental assessments of sites with unique environmental features or unique potential impacts are being used for several major proposed Air Force activities.

We are studying biodiversity and natural resources at a number of Air Force installations, focusing on the abundance of federal- and state-listed species and on the existence of exceptional natural communities. The information collected is incorporated into geographic information systems.

We also perform studies to identify for the Air Force the most cost-effective technical approaches to environmental management. For the Air Force Materiel Command, we are developing innovative approaches to computer-assisted management of large numbers of air pollutant emission sources in complex industrial areas. For the Air Force Center of Excellence, we are developing approaches for assuring that Air Force actions conform to state and local air quality maintenance strategies. New approaches to environmental management will shift the emphasis from compliance to pollution prevention. In addition, we are assisting the Pacific Air Force in its implementation of novel, cost-effective methods of carrying out environmental stewardship, including the management of cultural and natural resources at military installations in the United States and abroad.

We support a number of programs that serve Air Force Headquarters weather programs. For the Air and Space Natural Environment Executive Agent, we evaluate technologies and procedures for the Integrated Natural Environment Authoritative Representation Program. This program generates authoritative environmental

databases and models for use by the DOD modeling and simulation community. For the Air Force Combat Climatology Center, we are continuing our development of the Weather Effects for the Warfighter system, an operational planning tool for assessing the impact of the environment on military systems and operations. Also for the Combat Climatology Center, we are developing a cluster-based, mesoscale weather forecasting system for use in training and simulation. Simulated weather forecasts from this system will provide a rich training environment for staff weather officers.

As an extension of an earlier project, we are customizing an enhanced version of an advanced information tool to assist the Secretary of the Air Force, Office of the Inspector General, in handling requests made under the Freedom of Information Act. We are also conducting R&D on advanced battery technologies for the U.S. Air Force. This work includes fundamental investigations of the mechanisms for ion conduction in new battery materials and the design and optimization of battery cells based on these materials. We are also developing advanced materials for use in high-power rechargeable lithium batteries for aerospace applications. In other Air Force work, we have started a new program to investigate normal and superconducting radio frequency guns with tunable pulse compression.

## 2. The Joint Staff

We support the J-8 Directorate of the Joint Staff by evaluating emerging technologies and applying them to the mission challenges faced by the Joint community in the area of information management for modeling, simulation, and analysis. We help J-8 operations divisions conduct analyses more quickly and reliably by providing advanced simulation and analysis tools and methodologies. Key activities being supported include (1) validation and verification of data and models during the various phases of an analysis; (2) application of object-oriented and agent-based techniques to modeling and simulation; (3) information and knowledge management; (4) development of modeling and simulation architectures that provide

interoperability among legacy models, new models, and application packages; (5) development of logistics and deployment simulations; and (6) development of designs and applications for enhancing system security and evaluating new security technologies.

Analysis of logistics and mobility has become increasingly important to the U.S. military because of continuing rapid changes in the ways that forces are deployed. The objectives are lower costs, greater transparency, and more efficient management of the larger and more flexible logistic operations needed for modern warfare. Because more of the U.S. military is now stationed in the continental United States, greater importance is attached to contingency planning for deploying forces, both for missions such as disaster relief and peacekeeping and for military operations. Our work on logistics and deployment modeling and simulation has focused on four areas: developing prototype models and simulations, developing novel system architectures by integrating multiple model and simulation components, conducting technology feasibility studies, and providing technical guidance regarding technologies and systems designs.

The development of modeling and simulation architectures has been a primary focus of our work for the Joint Staff since 1987. One of the most useful results has been the Dynamic Information Architecture System (DIAS), an object-oriented simulation architecture capable of easily interfacing existing models and information processing applications. One notable application is an Integrated Ocean Architecture system that supports U.S. Navy operations.

Another major Argonne object-based framework, FACET (Framework for Addressing Cooperative Extended Transactions) supports the construction of models of complex, cooperative behavior by agents. FACET can be used to implement simulation models of organizational processes, such as the complex interplay of participating individuals and organizations engaged in multiple concurrent transactions in pursuit of their respective goals. Transactions can be patterned on, for example, business practices, government and corporate policies, military standard operating procedures and doctrine,

clinical guidelines, or office procedures. FACET can also incorporate other complex behaviors, such as biological life cycles or manufacturing processes.

For the Joint Staff, we are developing a tool that is being used to study interdiction strategies for countering the South American drug trade. The Complex Adaptive System Countermeasure Analysis Dynamic Environment-Counter Drug (CASCADE-CD) tool is intended to aid drug interdiction analysts in deriving and justifying force structure and operational planning recommendations. CASCADE-CD is an agent-based complex adaptive system simulation framework that models the trafficking aspects of the South American cocaine trade and the entire interdiction chain. Agents on both sides are provided with adaptive behaviors that are manifested at several scales and granularities.

### 3. U.S. Army

Argonne (in conjunction with DHS) assists the Army's implementation of the Chemical Stockpile Emergency Preparedness Program (CSEPP). The Laboratory supports program development, policy analysis and development of associated guidance, emergency preparedness planning, institutional analysis, development of hazard-specific risk communications and emergency public education mechanisms, and testing and assessment of response capabilities. We also assist in technical management. This work involves hazard analysis; modeling of chemical agent dispersion; development of cost estimation and measurement methodologies; integration of emergency planning; and collection, analysis, and validation of meteorological data at each CSEPP installation.

For the Operations Support Command, we are developing the Joint Munitions Planning System, a planning tool to support ammunition sourcing and movement strategies. This tool designs sourcing and movement strategies that best meet operational requirements established by battlefield commanders.

For the Army Environmental Center, we are conducting research at a series of demonstration sites to develop techniques for the environmental

characterization of contaminated installations and for monitoring *in situ* remediation in the continental United States. The research focuses on developing methodologies for characterizing groundwater pathways and delineating source terms and contaminant plume configurations that will serve as models for other installations, thereby expediting the selection of remediation technologies and the cleanup or closure of bases at many sites.

We also support the Army Environmental Center through R&D on environmental restoration at various Army installations, including several sites that have been placed on the National Priorities List. Specific activities include the development of state-of-the-art environmental data management systems to expedite remedial decision making and the use of groundwater and soil gas models to evaluate alternative methods of restoring aquifers. For the same sponsor, we support compliance and regulatory analyses, including critical issues related to military munitions and environmental management of military ranges.

Argonne helps the Army Corps of Engineers implement projects under Superfund and the Defense Environmental Restoration Program through the Savannah and Kansas City Districts. For the New York, Buffalo, and Omaha Districts, we are developing specialized approaches to remedial investigations and feasibility studies, particularly for sites having risk of radiological contamination and involving water resource restoration.

We assist several districts of the Army Corps of Engineers in the efficient execution of the Formerly Utilized Sites Remedial Action Program, which was transferred from DOE to the Corps in FY 1998. The specialized technical capabilities we bring to this cleanup program include the Adaptive Sampling and Analysis Program (ASAP), the RESRAD code for dose assessment, expertise in approaches specified in the *Multi-Agency Radiation Survey and Site Investigation Manual*, multiplatform geophysical characterization, and advanced tools for management of environmental data.

We are conducting an integrated program of environmental and engineering research and

technical support for the Army Corps of Engineers in the Baltimore and New England Districts and for the Army Environmental Center, examining issues such as land restoration, solid waste management, site characterization, detection of buried objects, and cleanup of hazardous waste sites.

For the Chemical Materiel Agency (formerly the Army Soldier and Biological Chemical Command), we assist in the development and analysis of restrictions regarding the land disposal of chemical agents and their by-products in the environment. Studies are coordinated with multiple environmental agencies within the Army and with several states. We also support the Command's Assembled Chemical Weapons Assessment Program in the area of environmental compliance for demilitarization of assembled munitions, by exploring alternatives to incineration of material from the U.S. chemical agent stockpile. For the Chemical Demilitarization Program, we investigate chemical methods for (1) analyzing agent standards and waste streams, (2) detecting heavy metals in waste streams, and (3) evaluating sampling methods. In addition, we are employing models and analyses to address environmental management issues at the Command's Rocky Mountain Arsenal, Pueblo Depot Activity, Tooele Chemical Agent Disposal Facility, and Aberdeen Proving Ground.

We provide technical assistance for environmental restoration activities at Aberdeen Proving Ground, which has a legacy of chemical contamination. We are seeking solutions to such problems through a restoration study at the J Field site and through sitewide remote sensing. Work addresses management of environmental information, wetlands issues, and the natural attenuation of groundwater contamination.

We have undertaken studies of the environmental risks posed by active and former test ranges for the Army Developmental Test Command. We are now conducting specific environmental restoration and compliance assessment studies at three installations of the Command (Dugway Proving Ground, Yuma Proving Ground, and White Sands Missile Range).

For the U.S. Army Defense Ammunition Center (USADAC), a part of the Operations Support Command (OSC), we are developing a data system for hazardous waste characterization to support environmental compliance related to the destruction of munitions and explosives at Army installations and to the reuse and recycling of components. In related efforts, we are developing a demilitarization planning and management system that incorporates the USADAC system and other information to improve the Army's ability to plan for cost-effective and environmentally sound demilitarization. In addition, we perform specialized environmental modeling and data analyses to address radiological risk and restoration problems at OSC installations (currently, at the Seneca Army Depot). We are also developing the Joint Munitions Planning System, an advanced technology simulation tool for managing the global distribution of munitions.

For the Army National Guard, we provide specialized technical assistance in the analysis of issues related to the environmental management of military ranges, evaluation of the performance of cleanup remedies, innovative site characterization, and modeling of groundwater.

We continue to use our DIAS simulation architecture to design and develop integrated modeling systems for installation management by the U.S. Army. The DIAS architecture is now being used for a new U.S. Army initiative called Fort Future, which will develop the capability to model, simulate, assess, and optimize installations that can support transformation of the Army to meet future needs. In particular, DIAS will be the model integration framework for simulating and optimizing force projection for Fort Future. The system will also contain an air dispersion model for analyzing force protection.

Also for the Army, we are developing biological microchips (biochips) for use as sensors and detectors. Custom chips for detecting biological agents are being tested around the country, and new technology for on-chip PCR (polymerase chain reaction) amplification of phylogenetic and functional gene target nucleic acids is under continued development. We are

developing methods of manufacturing biochips in enclosed flow cells and pursuing other advancements that will allow a single biochip to be used in the field for either custom analysis or PCR amplification.

#### **4. U.S. Navy**

We support the Naval Facilities Command (NAVFAC) and the Civil Engineer Corps Officer School in the area of ecological risk assessment, in part by transferring to the Navy restoration program the ecological risk assessment methodologies developed for DOE cleanup programs and also by developing information management systems to increase the efficiency of responses to ecological risk assessments. We also assess particular new cleanup methodologies and technologies. In addition, we provide technical leadership for NAVFAC's environmental characterization and risk assessment for depleted uranium at the Navy's China Lake facility. Investigation continues into decontaminating porous surfaces after contamination by dirty bombs. We are also continuing with the Infrastructure Assurance Technical Support Program for the Navy.

#### **5. Defense Threat Reduction Agency**

As part of an R&D program in support of arms control and homeland security, we develop treaty verification and threat attribution procedures and technology for the Defense Threat Reduction Agency. Currently, our verification programs focus on overall long-term information and organizational requirements for verification, validation, and compliance as additional treaties are being implemented. This activity includes analysis of functional requirements, technical evaluation, independent verification, and validation for new automated systems; prototyping for automated training techniques; and assistance in implementation planning. We also conduct life cycle analyses in support of strategic planning for arms control treaty software systems and perform studies and technical evaluations in support of the Open Skies Treaty. Recent additions to the homeland security component of this program include development

of methods and databases for attributing a domestic nuclear event to its perpetrators, training of ordinance disposal personnel in working with materials from radiological dispersal devices, and a project to evaluate and develop biochips for detecting and analyzing potential biological threats and exposure to biological agents.

#### **6. Defense Advanced Research Projects Agency**

For the Defense Advanced Research Projects Agency, we are developing oxide thin-film technology for radar and communications systems. We are also investigating toxin removal from the bloodstream by magnetic particles, as well as biomagnetic self-assembly with virus technology. Investigation continues into biochips for identifying pathogenic bacteria.

#### **7. Joint Program Office for Special Technology Countermeasures**

For the Joint Program Office for Special Technology Countermeasures, we are (1) identifying, collecting, and synthesizing data about the U.S. natural gas, petroleum fuels, and water infrastructures and (2) developing and applying analytical tools for isolation and system analyses. In addition, we are examining trends in the petroleum refining industry, modeling infrastructure interdependencies as complex adaptive systems, and examining risk-based decision methodologies. The overall objective is a capability to identify susceptibilities and operational dependencies in critical infrastructure that, if not remedied, could threaten accomplishment of vital military missions.

### **C. Department of Health and Human Services**

Funding for our work for the Department of Health and Human Services either flows through the University of Chicago or is received directly through interagency agreements with DOE. (In Chapter VI see University of Chicago Grants and

Department of Health and Human Services, respectively.)

#### *University of Chicago Grants*

The National Institutes of Health (NIH) supports a broad range of fundamental studies at Argonne. These investigations often apply techniques developed in DOE-supported programs to studies in structural biology, biophysics, carcinogenesis, mutagenesis, and physiology. In turn, our work for NIH bolsters our resources for addressing the DOE science mission, including the DOE Genomes to Life program. Most of our studies for NIH emphasize structure-function relationships or mechanisms underlying biological responses.

Our biophysics studies for NIH are addressing the properties of human antibody light chains that lead to pathologic deposition in myeloma. Investigations of *in vitro* aggregation of light chains consider their structure and pathologic characteristics. For example, one project is developing new procedures for the heterologous expression of functional membrane proteins in quantities sufficient for x-ray crystallography to determine the proteins' structures and functions.

We are among the initiators of the U.S. structural genomics program. NIH now is supporting a major effort in structural genomics at Argonne, with an ultimate goal of determining the structures of all protein families. This effort for NIH, in partnership with the DOE-funded Structural Biology Center (SBC) at the Advanced Photon Source (APS), created the Midwest Center for Structural Genomics (MCSG). Argonne is the lead institution in the MCSG consortium, which also includes six universities. NIH will provide approximately \$7 million annually through FY 2005 to establish high-throughput methods for determining the three-dimensional structures of proteins from bacteria and higher eukaryotes. As recently as 1990, solving a single protein crystal structure could take one or more scientists several years. At Argonne, improved techniques for data collection, analysis, and structural determination now allow the structure of a protein to be solved in as little as six hours. Using x-rays from the APS, the SBC collects data of very high quality, significantly faster than was possible even a few

years ago. By developing (1) robotic methods to carry out tedious experimental procedures and (2) advanced computational methods for data analysis and structure determination, we have achieved huge leaps in productivity. The MCSG is continuing to develop high-throughput methods in molecular biology, protein purification, and crystallization. Combined with highly efficient SBC beamlines and automated crystallography, these methods will further accelerate the process of determining new protein structures. The NIH support of the MCSG will enable further major improvements in productivity.

We are collaborating with the University of Chicago Medical School to develop an ice slurry treatment that will decrease cell death due to reduced blood flow and oxygen availability after cardiac arrest or stroke. A medical-grade slurry is used to cool the brain and heart rapidly and induce hypothermia. NIH recently funded a five-year project for further development of the coolant and associated clinical procedures.

In other work, NIH supports Argonne's development of models that simulate turbulence in the carotid artery. This effort, conducted by Argonne computer scientists in collaboration with researchers at the University of Illinois at Chicago and the University of Chicago, aims to help physicians make treatment decisions tailored to individual patients.

For NIH we are developing a new technology for rapidly detecting and characterizing pathogens in the environment, even before the onset of clinical symptoms. This technology will use the integrated three-dimensional gel pad microchip mentioned earlier for sample purification, amplification, and detection.

We will contribute to improving national defense against biological warfare as a member of the NIH-funded Midwestern Regional Center of Excellence for Biodefense and Emerging Infectious Diseases Research (RCE). This multidisciplinary, multisite effort focuses on the diseases anthrax, botulism, hemorrhagic fever, plague, and tularemia. Led by the University of Chicago and Northwestern University, the RCE involves multiple universities, research institutes, and public health authorities and, altogether, more than 100 scientists — including several from

Argonne. Central objectives are to improve basic understanding of the diseases' pathogenesis, create novel therapeutics, develop vaccines or other preventive strategies, and develop better diagnostic technologies. Argonne is proposing projects to investigate (1) whether genetic determinants essential to the pathogenesis of anthrax disease can serve as targets for therapy; (2) bioinformatics analysis of certain important genomes, along with metabolic and pathogenic reconstruction; (3) use of affinity imprinting to develop a new system for detecting hemorrhagic fever viruses; and (4) development of a powerful data analysis and computational environment for use by RCE participants. In addition, the Laboratory is to contribute to overall administration of the center.

To support the RCE, a Regional Biocontainment Laboratory (RBL) is to be built at Argonne through a University of Chicago program supported by NIH. This laboratory will provide RCE researchers with facilities certified to "biosafety level 3" (the third highest of four levels). Placing the RBL at Argonne will ensure ready access to complementary Argonne facilities such as the APS, the SBC, the MCSG (with its focus on rapid selection, robotic generation, purification, crystallization, and structural analysis of proteins), the Mathematics and Computer Science Division (for information analysis and modeling), and the Center for Nanoscale Materials.

#### *Interagency Agreements with DOE*

Another NIH partnership with Argonne aims to construct and operate a new collaborative access team (GM/CA-CAT) at the APS. This effort will pursue parallel cooperative work with the SBC and the MCSG. Using two undulators and a bending magnet, GM/CA-CAT will develop three x-ray beamlines optimized for macromolecular crystallography. A new office-laboratory module is providing office and laboratory space for staff and users. The beamlines will include high-throughput robotic sample delivery, high-speed data collection with online analysis, and remote access through interactive computer networks. Construction of the beamlines, begun in FY 2003, will proceed in sequential phases that will allow data collection

to begin at the first beamline during construction of the other two beamlines.

Argonne provides technical support to the U.S. Public Health Service, Division of Federal Occupational Health, in the development and implementation of an environmental health and safety assessment program for the U.S. Social Security Administration. The principal objective is to develop an overall program framework, plans and protocols, and facility assessments at randomly selected facilities in ten regions. Information gathered during pilot assessments in a few regions will be used to guide subsequent work.

## **D. Other Federal Agencies**

### **1. Environmental Protection Agency**

For the U.S. Environmental Protection Agency (EPA), we apply our DIAS architecture as the framework for ecosystem modeling and environmental health assessment through an EPA system known as MIMS (Multimedia Integrated Modeling System). MIMS allows researchers to consider the environment for nutrients and chemicals across air, water, and land. We are also helping the EPA develop a prototype multicompartment model within MIMS.

For the EPA Office of Pollution Prevention and Toxics and EPA Region V, we are extending methods of analyzing cumulative environmental risks in urban areas by enhancing the availability and performance of scientifically sound procedures, models, analytical tools, and guidelines. One objective is to identify areas within the metropolitan Chicago region where exposures of the general population to individual pollutants or combinations of pollutants might be significant.

For the EPA Office of Research and Development (ORD) at the National Center for Environmental Assessment, we are evaluating and implementing methodologies related to assessing cumulative risks, including risk of exposures to chemical mixtures by multiple pathways. Applications to DOE sites are being demonstrated. For the National Homeland Security Research Center at EPA-ORD, we are

developing rapid risk assessment methods and short-term health advisory levels.

We will assist the EPA Technology Innovation Office with its Triad Program of systematic planning, dynamic work plans, and field analytics. This effort aims to accelerate environmental cleanup by employing Argonne's experience with adaptive sampling, expedited characterizations, and brownfield sites. Included is support to EPA regional offices.

For the EPA Office of Radiation and Indoor Air, we are assisting in the evaluation of technologies and methods for detecting and analyzing radioactive contamination in imported scrap metal. A pilot study at the ports of New Orleans and Charleston included deployment of a detection system and analysis of imported scrap metal.

For the EPA Office of International Activities, we are evaluating thermal destruction technologies to treat persistent organic pollutants, including polychlorinated biphenyl compounds and obsolete pesticides. The technology is to be demonstrated in the Russian Federation. Results are expected to benefit DOE sites directly.

The EPA's National Risk Management Research Laboratory is supporting development of instrumentation for the proposed EnviroCAT beamline at the APS. (See the Challenges in Environmental Science initiative in Section IV.A.9.) Representatives of the EPA laboratory participate in the EnviroCAT Founding Member Institutions group and are to be actively engaged in all phases of the EnviroCAT project. The EPA's objective is to help design instrumentation that exploits the unique x-ray beams produced by the APS insertion device. The focus is on a new microprobe combining, in a single device, Fresnel zone plate and Kirkpatrick-Baez mirror optics. This approach will extend the operating spatial resolution range from below 0.1 micrometer to about 100 micrometers. The resulting instrument will be able to analyze individual samples over this broad resolution range, with resolution adjustments in pseudo-real time. Such a capability is crucial in speciation studies of highly heterogeneous environmental materials such as contaminated soils.

For the EPA Office of Air and Radiation, we are studying the fuels infrastructure needed for fuel cell vehicles. We are also incorporating our GREET (Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) model into the EPA's new generation of transmission emissions models.

## **2. Department of State and International Atomic Energy Agency**

Throughout most of its existence, Argonne has actively supported the worldwide transfer of peaceful applications of nuclear technology. Shortly after the Laboratory was founded, its first international training activities were established as part of the Eisenhower Atoms for Peace program. Participants came from throughout the world to learn about the new, rapidly developing field of nuclear reactor technology. In many countries, graduates of these programs are today the leaders of national programs involving the peaceful applications of nuclear technology.

In 1976 we were designated by the Department of State as host institution for U.S. participation in the new Nuclear Power Training Program of the International Atomic Energy Agency (IAEA). Under this program we today continue to develop, organize, and conduct training courses covering a full range of topics in the peaceful applications of nuclear technology. Subject areas include nuclear safety, security and research reactor safety, D&D, energy planning, isotope hydrology, and medical physics. Approximately 3,300 professionals from over 121 countries, representing essentially all developing member states of the IAEA, have received intensive training through these courses.

We provide technical and management support to the Department of State and directly to the IAEA. One major activity is evaluation of technical cooperation projects proposed for funding by the United States, along with monitoring and facilitation of the implementation of such projects once funded. We developed and now maintain — by means of an electronic database — an “institutional memory” of U.S. support for technical cooperation projects, as well as extensive project files, IAEA reports, and evaluation studies. We also support the

Department of State and the IAEA in their initiatives to improve the agency's technical cooperation program. Argonne regularly reviews and analyzes the program's management and achievements. We also develop recommendations on matters of policy or practice related to U.S. support for the program. By providing experts for technical cooperation programs, Argonne has helped many countries develop the ability to analyze the operation of their energy systems.

We also support the Department of State each year by placing nearly 150 IAEA fellows at research institutions throughout the country for periods up to six months.

### **3. Department of Transportation**

For the Research and Special Projects Administration, we continue to model the effects of accidents resulting from transportation of chemicals on the nation's highways and railways. These models will address (1) the effectiveness of establishing protective distances from accidents involving spills on highways and rails and (2) chemical spills into bodies of water from highway and rail accidents. In support of regulation development, the Laboratory is involved in a national assessment of risks (especially risks through inhalation) associated with transporting toxic chemicals.

### **4. Department of Agriculture**

As part of an ongoing program for the Commodity Credit Corporation of the U.S. Department of Agriculture (CCC/USDA), Argonne supports remediation of sites having contaminated groundwater and soil by integrating field sampling, groundwater modeling, and engineering cost analyses. We are also developing new cone penetrometer technologies and using them — in combination with innovative sampling, analytical, and computer data processing methods — to map the subsurface distribution of contaminants in soils and groundwater at former CCC/USDA grain storage sites. In addition, we are conducting pilot studies of spray irrigation as an alternative to traditional methods of treating contaminated groundwater.

We are assisting in the technical development of the Research, Education, and Economics Information System (REEIS), a "data mart" that integrates multiple databases in the USDA's Research, Education, and Economics program by using a web-based information architecture. REEIS will improve access to information by employing a consistent, integrated framework and will provide automated tools for analyzing the information.

The U.S. Forest Service, DOE's Argonne Site Office, and Argonne have signed a master interagency agreement that facilitates the use and application of Laboratory technical resources to support management of the nation's forests and grasslands.

### **5. National Science Foundation**

Funding for most Argonne work for the National Science Foundation (NSF) flows through universities (see Chapter VI).

We are a partner in the National Computational Science Alliance, funded by the NSF Partnerships for Advanced Computational Infrastructure (PACI) program. Researchers are developing software for collaborative problem solving, distributed computing technology, advanced visualization tools, and parallel input-output technology.

We are one of five institutions participating in the TeraGrid project, which aims to develop the world's first multisite supercomputing system, the Distributed Terascale Facility. The TeraGrid is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign and by the San Diego Supercomputer Center, two leading PACI sites. By integrating the most powerful computers, software, networks, data-access systems, and applications, the TeraGrid will create a unique national resource to support scientific breakthroughs.

As a world leader of emerging grid technologies, we collaborate on several NSF-funded projects, including the Network for Earthquake Engineering Simulation project with the NCSA; the GRIDS Center project with the

University of Chicago, the University of Southern California Information Sciences Institute, the University of Illinois at Urbana-Champaign, and the University of Wisconsin; and the Grid Physics Network project with more than two dozen U.S. universities.

We are also pursuing several smaller computer science projects funded by NSF, including development of extensible network services for the Access Grid and design of adjoint compiler technology.

We are collaborating with other NSF projects to develop the National Science Digital Library. In particular, under NSF funding we are leading Eastern Illinois University and the University of Utah in producing a digital library collection that improves the accessibility and usability of DOE Atmospheric Radiation Measurement Program data for the education and research communities.

## **6. National Aeronautics and Space Administration**

For the National Aeronautics and Space Administration (NASA), Argonne is developing test beds to study applications of distributed computational grids. Argonne researchers, together with investigators at the University of Southern California's Information Sciences Institute, are also teaming with NASA researchers to implement Globus Toolkit<sup>®</sup> technology for linking the computers on the NASA Information Power Grid.

In addition, Argonne is building a state-of-the-art laboratory for trace element detection to study the composition of interstellar dust from supernovas and from comet tails, as well as the compositions of components of the solar wind retrieved from Earth satellites. These studies will reveal secrets of the origin and evolution of the universe.

In other work for NASA, Argonne is providing technical assistance and oversight for the Plum Brook Reactor Facilities Decommissioning Project. Five Argonne staff members are serving in the areas of management of construction, quality assurance, health and safety, radiation safety, licensing, and regulatory

compliance. This project is expected to continue until 2007.

For use in advanced propulsion systems and outer shells for high-speed aircraft, NASA is investigating advanced ceramic composite materials. In support of this effort, we are developing noncontact, nondestructive test methods to determine the condition of the materials before, during, and after a test cycle.

## **7. Department of Commerce**

Argonne works with two organizations within the Department of Commerce: the National Oceanic and Atmospheric Administration and the National Institute of Standards and Technology (NIST).

The NIST Advanced Technology Program requires participating private companies to match NIST funding. The private sector can then choose to subcontract to the national laboratories in the pursuit of new technology.

## **8. Department of the Interior**

We provide technical support on environmental issues to the Bureau of Land Management (BLM) of the Department of the Interior, helping the BLM maintain long-term stewardship of public lands while allowing production of resources such as oil and natural gas.

We are funded directly by DOE to support BLM energy planning in the Farmington (New Mexico) and Worland (Wyoming) field offices. These projects test new tools designed to enhance data sharing and provide baseline measurements needed for energy development. In addition, we have conducted several technical studies. For the BLM we also recently began work on the North Slope Science Initiative, which will support resource management on the North Slope of Alaska by integrating inventory analysis, monitoring, and research.

For the Fish and Wildlife Service, we develop environmental information and communications systems. One of the systems is being developed jointly with the Chicago Wilderness Society.

For the Bureau of Reclamation we provide technical support on the management of hydropower. We evaluate the impacts to water quality and aquatic ecosystems from modification of water use in the Klamath River basin; identify and evaluate environmental and security issues associated with strategies for increasing U.S. hydropower production; and analyze technical and environmental issues associated with international hydropower agreements.

## E. Nonfederal Organizations

### 1. Electric Power Research Institute

Argonne conducts research for EPRI on topics related to the risk of a severe accident at a nuclear power plant. Research for the MACE program was particularly important. This work investigated the ability of water to quench and cool a pool of molten core debris without formation of a continuous insulating crust, thereby terminating an accident and preventing basemat penetration. The investigations attracted worldwide attention because of their importance to strategies for managing accidents at existing plants and their great relevance to design decisions for future light-water reactors. These experiments were sponsored by the 15-nation Advanced Containment Experiments program headed by EPRI, which pursued realistic understanding of the consequences of an accident involving core melting. A successor to the MACE program is now being conducted under the sponsorship of the Organization for Economic Cooperation and Development. (See discussion of the Melt Coolability and Concrete Interaction program in Section S1.E.5.)

Complementary Argonne programs for EPRI aim to resolve key safety issues through a combination of analysis and experiments. The computer code CORQUENCH, based on data from Argonne experiments, is being used to analyze accident phenomena.

Other work for EPRI includes identifying and characterizing technologies and processes for mitigating the environmental impacts of cooling water at electric power plants. We also assess the

use of these technologies and processes in innovative approaches to meeting environmental regulations.

### 2. Private Organizations

We conduct research for a number of private firms and other private organizations, giving them access to our unique facilities and technical resources. Current work includes the following:

- Air Products, Inc.: Development of an advanced electrolyte system with viscosity and high conductivity suitable for high-power lithium batteries containing spinel-based cathodes.
- Aramco Services Co.: Assessments of alternatives for disposing of naturally occurring radioactive material, including analyses of potential radiological risks and relative costs.
- BASF Corp.: Production of specialty chemicals in pilot plant quantities to test a new electro dialysis process.
- Battelle Memorial Institute: Forensic identification and diagnosis of *Bacillus anthracis*, demonstration of a universal DNA fingerprinting microarray, and automated image and data analysis algorithms.
- California Energy Commission: Research on an advanced laser ignition system for use in stationary reciprocating engines fueled by natural gas, a technology that could improve engine efficiency, emissions performance, maintenance costs, and frequency of replacement.
- Climax Molybdenum: Development of hydrosulfurization catalyst materials.
- Duke Cogema Stone & Webster, LLC: Investigation to help characterize any risk of plutonium third-phase formation in solvent extraction systems, in support of the design of the Mixed-Oxide Fuel Fabrication Facility to be constructed at the Savannah River Site.
- General Atomics: Development of a tile computer display wall.

- General Motors Electro-Motive Division: Improvement of the efficiency and emissions characteristics of diesel engines.
- IBM: Development and implementation of the Open Grid Services Architecture, a set of specifications and standards that will combine the benefits of grid computing and web services.
- Intel Corp.: Exploration of extreme ultraviolet lithography through consideration of conceptual designs, innovative physics, and plasma-material interactions.
- Procter & Gamble: Agent-based modeling and simulation techniques to model consumer goods markets.
- Quallion, LLC: Development of advanced lithium batteries for soldiers' "power vests." (Funding is from the U.S. Army Communications and Electronics Command.)
- Quallion, LLC: Development of a rechargeable miniature battery to power implantable microstimulators that could help millions who suffer from neurologic disorders such as urinary urge incontinence.
- Solar Turbines, Inc.: Application of new nondestructive evaluation technologies to ceramic materials being developed for gas-fired turbine engines that emit less pollution and operate more efficiently.
- Thermoelectrica Co.: Revision to an environmental assessment for permit applications by Baja California Power, Inc.

In addition to the activities administered under Argonne's WFO program, as discussed in this Supplement 1, the Laboratory also performs work with its partners in cooperative R&D agreements. These activities are discussed in Supplement 2.

Argonne's work for private firms often grows out of industry-laboratory collaborative projects. A good example is our Laser Applications Laboratory, which conducts R&D to support the use of high-power lasers. Projects typically relate to materials processing for manufacturing (such as laser heat treatment of casting dies) and to new uses (such as drilling wells with lasers). Processing techniques available at the Laser

Applications Laboratory include high-power beam shaping and delivery, fiber optics, surface modification, and welding. Industrial partners include automotive manufacturers and suppliers and also several small businesses. One example of benefits to private firms is a low-cost weld monitor being used in a DaimlerChrysler plant in Kokomo. This monitor has saved millions of dollars by improving weld quality. Work by the Laser Applications Laboratory generally supports Argonne's major facilities and programs, such as the APS, the Intense Pulsed Neutron Source, the fusion power program, and D&D of reactor systems.

### 3. Universities

Current Argonne work for universities includes the following:

- Northern Illinois University: Collaboration on the development of MPICH-G2, a grid-enabled implementation of the Message Passing Interface standard for communications between machines having different architectures.
- Northwestern University: Educational outreach to place Illinois undergraduate students in summer research participation positions at the APS.
- University of Alabama: For several hydrogen-based technologies, establishment of baseline data from a series of experiments, tests, and evaluations.
- University of Alabama: Development and characterization of fuel cell components for automotive fuel cell systems.
- University of Alabama-Birmingham: Modeling and simulation of fuel cell systems.
- University of Chicago: Collaboration on the Grid Physics Network project in the areas of data grid and virtual data research, toolkit development, application challenge problems, and outreach.
- University of Chicago: As part of the Illinois Consortium of Accelerator Research project, technical support involving theoretical and simulation analysis of beam dynamics

problems that are critical for the performance of linear colliders.

- University of Illinois at Urbana-Champaign: The Partnership for Advanced Computational Infrastructure program.
- University of Illinois at Urbana-Champaign: Assistance in developing middleware communication services for grid-based collaborations for the project Network for Earthquake Engineering Simulation.

#### 4. State and Local Government

For the Illinois Commerce Commission, we are analyzing the state's electric power transmission system by using a new modeling and simulation approach we developed to study complex adaptive systems.

For the California Energy Commission, we are conducting research on laser-based ignition systems for use in stationary reciprocating engines fueled by natural gas, a technology that could eliminate the high maintenance and replacement requirements of conventional spark plug systems.

State groundwater regulatory agencies are prominent members of the nonprofit Ground Water Protection Council, along with federal agencies and other parties interested in protecting the nation's groundwater supplies. Argonne's work for the council involves preparing environmental analyses and developing environmental information management systems, all with a focus on the relationship of energy systems to groundwater protection.

For the Washington Metropolitan Transit Authority, we are providing technical support for development of a chemical agent early warning system.

#### 5. International Organizations and Foreign Countries

With the World Bank and countries borrowing from the Bank, we are working on energy and environmental analyses addressing issues such as planning least-cost expansions for

electrical generating systems, estimating marginal costs of electricity production, simulating the operation of mixed hydrothermal systems, projecting overall energy supply and demand, analyzing current and future environmental effects of energy production and consumption, estimating the potential for future pollution abatement projects and their costs, and estimating the costs and effects of greenhouse gas mitigation options. We typically conduct these studies in close cooperation with experts in the borrowing countries, who often are trained to use the analytical techniques themselves.

To advance nuclear reactor technology, international sponsors use Argonne's unique capability to perform severe-accident experiments with real reactor materials. We currently work with Atomic Energy of Canada, Ltd., on an experiment to explore molten fuel-fluid interaction for the CANDU reactor. We are conducting other accident-related research as part of the Melt Coolability and Concrete Interaction program sponsored by the Organization for Economic Cooperation and Development. The technical objectives of this multiyear program are to investigate the mechanisms by which debris cools outside the containment vessel and to address remaining uncertainties related to long-term, two-dimensional interactions between the reactor core and concrete. These objectives will be met through a series of experiments and associated analyses.

In other work, the Japan Nuclear Cycle Development Institute supports studies of the operational characteristics of reactor concepts, the safety testing needed for advanced fuels, and the irradiation behavior of materials. The Central Research Institute of the Electric Power Industry of Japan also supports studies of the irradiation behavior of structural materials. Argonne collaborates with the Korea Atomic Energy Research Institute (KAERI) on several aspects of nuclear reactor technology, safety research, and advanced computing applications. We are also working with KAERI on International Nuclear Energy Research Initiatives (1) to evaluate structural materials for use in the pyrochemical processing of spent nuclear fuels and (2) to evaluate and develop materials for use in Generation IV supercritical-water reactors.

We work directly with many foreign countries to provide energy and environmental analyses, along with training in the use of supporting computer models. Included are Argonne's ENergy and Power Evaluation Program (ENPEP) and Generation and Transmission Maximization (GTMax) models.

In a major project, we work with countries in eastern Europe (Romania, Bulgaria, Macedonia, Albania, Serbia, Montenegro, Croatia, and Bosnia-Herzegovina) to analyze the operation of their electric power systems as integrated entities rather than as separate systems. The objective is improving economic and operational efficiency. The project involves the U.S. Agency for International Development and the World Bank.

Argonne is the operating agent for the International Energy Agency program Implementing Agreement for a Co-Operative Programme for Assessing the Impacts of High-Temperature Superconductivity on the Electric Power Sector. The Laboratory's main role is to keep member countries informed about the status of superconductivity research and its progress toward application. The implementing agreement is funded by organizations in 16 countries, including the United States.

We are collaborating with researchers at the European particle physics center at CERN on the DataGrid Project, which aims to build the next-generation computing infrastructure for computation and analysis of petabyte-scale databases by widely distributed scientific communities. This work will build on technologies developed by Argonne's Globus Alliance. Researchers in the Globus Alliance are also working with the Poznan Supercomputing and Networking Center in Poland to develop GridLab. Globus Toolkit<sup>®</sup> services and libraries, such as GridFTP and Globus Resource Allocation and Management, will be used to support the development of dynamic grid-enabled applications.

The International Energy Agency has established international collaboration agreements on transportation fuel cells and on polymer electrolyte fuel cells under its Implementing Agreement on Advanced Fuel Cells. In both cases Argonne serves as operating agent, performing

fuel cell research, coordinating information flows, and conducting international meetings.

## **F. Department of Homeland Security**

Argonne conducts research for several DHS organizations on essentially the same basis as for DOE.

### **1. Information Assurance and Infrastructure Protection**

For the High Value and Soft Targets Unit of the DHS Information Assurance and Infrastructure Protection (IAIP) office, we produce background information on critical infrastructure facilities, participate in site assistance visits, integrate reports, implement and update vulnerability databases, develop common vulnerability expertise, and provide training.

We support vulnerability assessment efforts of the IAIP's Standards and Methodology Unit by identifying vulnerability assessment needs, collecting assessment methodologies, coordinating methodology development, assisting in setting standards for methodologies, and coordinating and evaluating methodologies for public and private entities. We are also coordinating and refining DHS methodologies.

For the IAIP's Protective Measures Section, we participate in visits to assess the protection afforded by buffer zones, provide expertise on infrastructure systems and interdependencies, and help with technology assessments.

### **2. Science and Technology**

Within the Critical Infrastructure Protection Portfolio of the DHS Science and Technology (S&T) office, we are partnering with Los Alamos National Laboratory and Sandia National Laboratories to develop a risk-based Critical Infrastructure Protection Decision Support System that provides insights for improving decisions related to protection of critical infrastructures. The system considers all

14 critical infrastructures and their primary interdependencies.

We also are conducting research for S&T's Biological/Chemical Portfolio. One project involves developing a system for the forensic identification of bioagents or pathogens disseminated in the environment, in host vectors, or in the populace. The system employs a universal DNA fingerprinting chip, instrumentation analysis software, and the statistical basis for identifying bioagents or pathogens without prior knowledge of their genomes or DNA sequences. A second project is developing a decontamination process for sensitive equipment and other applications that is to be effective against both chemical and biological agents. Approaches being considered are a gas-phase process using ultraviolet light and ozone and a liquid-phase process using ultraviolet light and peroxide.

We have been asked to work with S&T's Radiological and Nuclear Portfolio. The work scope, which is still being determined, is expected to include efforts in the passive detection program, in refining the analysis of needs and technical approaches for active detection, and in the Predetonation Attribution Program for radiological dispersal devices.

### **3. Federal Emergency Management Agency**

Our support to the Federal Emergency Management Agency involves three major areas relating to accidental or deliberate releases of chemical, biological, and radiological materials: (1) analysis and evaluation of the capabilities of U.S. industry, nearby communities, and host

states to respond to emergencies involving the materials; (2) R&D on guidance for emergency planning, exercises to test emergency plans, and response activities; and (3) the development and conduct of training activities.

### **4. Other DHS Areas**

We support the DHS Office for State and Local Government Coordination and Preparedness (formerly the Office for Domestic Preparedness) through planning support under the Urban Areas Security Initiative, development and implementation of the Homeland Security Exercise and Evaluation Program, and development of automated tools for designing exercises. Future efforts will include supporting the Top Officials (TOPOFF) Exercise 3, integrating automated planning and exercise tools into a homeland security toolkit for state and local governments, and designing a national program of homeland security exercises.

For the same office we are conducting the PROTECT program, which aims to improve rapid response to chemical attacks in the Washington, D.C., subway system. We are expanding the scope of the program, improving its robustness and redundancy, and decreasing its maintenance costs.

We await the signing of an interagency agreement between DHS and the Transportation Security Administration (TSA) that will serve as the contractual vehicle under which we work on a biochip program for TSA. This agency has also asked us to develop two white papers on radiation detector technology for use in railway stations and metropolitan subway stations.



# Supplement 2: Technology Transfer

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Argonne interacts extensively with researchers from industry, academia, and not-for-profit organizations in pursuit of the Laboratory's technology transfer objectives. We focus on providing technical solutions to challenges in the fields of energy, the environment, transportation, information, materials, and the life sciences. These interactions, in most cases conducted under formal R&D agreements, enhance Laboratory programs and provide a means of transferring into use the technologies and methodologies created by Argonne researchers. These interactions ultimately enhance U.S. economic productivity, international competitiveness, and society as a whole.

## A. R&D Agreements

Argonne's Office of Technology Transfer (OTT) is responsible for a broad range of activities. The office's overall objective is to increase the impact of the Laboratory's research, particularly by expanding use of its R&D results. OTT (1) manages the development of R&D agreements, including cooperative R&D agreements (CRADAs) and "work-for-others" (WFO) contracts; (2) seeks opportunities to increase collaboration with the University of Chicago; (3) develops partnerships with industry; (4) licenses intellectual property; and (5) serves as a point of contact for outreach activities and for incoming inquiries. Table S2.1 summarizes Argonne's technology transfer activities for FY 2001–FY 2003 and projects those activities for the subsequent three years.

Staff of OTT work closely with Argonne research divisions to develop new contract activities efficiently and to identify strategically important technology transfer opportunities with potential for high market impact. In these efforts, OTT staff are extensively involved in the Argonne Partnerships Committee, under whose auspices research managers meet regularly in tactical working groups to explore opportunities for

transferring technology to industry and to identify promising R&D programs of programmatic and commercial importance. The tactical working groups coordinate opportunities in five focus areas: (1) transportation technology, (2) environment and urban technology, (3) hydrogen technology, (4) materials technology, and (5) biotechnology.

Argonne research staff and OTT managers aggressively develop joint research programs and other collaborations with non-DOE organizations. They also work with the Laboratory's operating contractor, the University of Chicago, to use the resources and facilities of both institutions more effectively.

## B. Licensing

For Argonne inventions thought to have the greatest commercial potential — on the basis of their benefit to users, their commercial value, and the strategic need served — OTT works with research divisions to develop market-based technology commercialization strategies. In assessing commercial potential, we compare economic value with current alternatives and consider market size, cost of implementation, industry trends, and customer need for the technology. Through various kinds of cooperative agreements, Argonne collaborates with industrial firms to find the shortest, most effective route to technology commercialization and wide market adoption.

Table S2.1 reports royalties and other income received from licensing Laboratory inventions. Royalties received to date are from (1) up-front payments for licenses, options, and assignments and (2) current licensing agreements and royalties for ongoing sales of products and software. Income resulting from the commercial use of an Argonne technology is shared between its inventors or authors and the research divisions from which the technology originated. The divisions can use the funds for internally

Table S2.1 Activities Conducted by Argonne's Office of Technology Transfer

	Actual Values			Projected Values		
	FY 2001	FY 2002	FY 2003	FY 2004	FY 2005	FY 2006
<b>Office of Technology Transfer</b>						
Funding (\$ in millions)	2.3	2.0	2.0	1.95	1.95	1.95
Staffing (FTEs)	16	16	17	16	16	16
<b>Active Agreements (including amendments)<sup>a</sup></b>						
Cost-shared contracts (CRADAs)	27	32	30	26	24	24
Work-for-others contracts (research and technical service agreements)	246	248	209	256	300	300
Reimbursable work for the Department of Homeland Security	-	-	9	15	25	25
Work for other DOE contractors	351	349	389	350	390	390
Total	624	629	637	647	739	739
<b>Agreement Funding (funds to the Laboratory, \$ in millions)<sup>a</sup></b>						
Cost-shared contracts (CRADAs)	12.1	5.0	3.4	5.5	6.0	6.5
Work-for-others contracts (research and technical service agreements)	70.0	89.7	108.0	117.0	121.0	121.0
Reimbursable work for the Department of Homeland Security	-	-	6.6	19.0	21.0	25.0
Contracts with other DOE contractors	35.3	49.9	32.7	39.0	42.0	42.0
Total	117.4	144.6	150.7	180.5	190.0	194.5
<b>Intellectual Property</b>						
Inventions reported	106	106	118	140	150	150
Software reported	17	7	12	12	15	15
Patent applications filed <sup>b</sup>	49	50	56	50	75	75
Patents issued <sup>b</sup>	46	28	51	36	40	40
Patent inventory <sup>c</sup>	148	168	202	225	247	268
Active licenses (all sources) <sup>d</sup>	121	178	190	205	240	285
Royalties (gross, \$ in millions)	2.4	2.5	2.2	2.2	1.5	1.7

<sup>a</sup> Includes agreements with both nonfederal and federal organizations.

<sup>b</sup> Includes (1) patent applications filed by Argonne, ARCH Development Corporation, DOE, and others (e.g., inventors and companies) and (2) patents issuing from those filings.

<sup>c</sup> Excludes patents issued by Argonne but turned over to and maintained by others, such as ARCH Development Corporation or DOE.

<sup>d</sup> Includes licenses executed by Argonne, ARCH Development Corporation, and DOE.

supported R&D, staff development or educational activities, and technology transfer (under policies set in accordance with the *Prime Contract*).

Argonne licenses copyrighted software codes and accompanying documentation to commercial and educational organizations for a fee. In some cases, selected software is distributed broadly under free licenses to maximize market impact and overall benefit to users. The Laboratory also registers trademarks associated with its software and some elements of its invention portfolios, in order to distinguish and protect intellectual property reported in scientific journals, trade publications, and other venues.

The following currently available software packages are enjoying significant use:

- **EMCAS:** The new-generation EMCAS (Electricity Market Complex Adaptive System) modeling and simulation code for the electric power industry (URL: [www.anl.gov:80/PA/logos20-3/cass01.htm](http://www.anl.gov:80/PA/logos20-3/cass01.htm)). EMCAS is based on complex adaptive system technology that Argonne pioneered. EMCAS was recently licensed to Adica Consulting, a small start-up consulting and software distribution firm.
- **ERSM:** The software tool ERSM (Emergency Response Synchronization Matrix) for emergency managers. ERSM helps to develop crisis plans that coordinate actions across jurisdictions and over an extended time horizon, so that responders can coordinate effectively (URL: [www.anl.gov:80/OPA/news03/news030404.htm](http://www.anl.gov:80/OPA/news03/news030404.htm)).
- **GTMax:** The software package GTMax (URL: [www.techtransfer.anl.gov:80/highlights/9-3/gtmax.html](http://www.techtransfer.anl.gov:80/highlights/9-3/gtmax.html)) for power utilities. GTMax helps operators of thermal and hydropower generation facilities optimize their use of resources. Adica Consulting is promoting GTMax through international development organizations such as the World Bank, the United Nations, and the Japanese Development Bank, as well as through direct contacts with developing countries and strategic engineering firms. In 2003 Adica received the Federal Laboratory Consortium Midwest Region Industry/Non-Federal Government University Award for its efforts to commercialize GTMax.

- **LDAP Browser/Editor:** Argonne's LDAP Browser/Editor (URL: [www.softwareshop.anl.gov/ldapbrowser.html](http://www.softwareshop.anl.gov/ldapbrowser.html)) for modifying the contents of LDAP databases and configuring different editors or viewers. The LDAP Browser/Editor is independent of vendor and platform and has a user friendly graphic interface. (The popular web-based LDAP [Lightweight Directory Access Protocol] standard is used to access computerized directories that store and retrieve information.) In the 1999 Novell Developer Contest, LDAP Browser/Editor won the Student Application Grand Prize.

- **PSAT-NP:** Argonne's PSAT-NP program (Powertrain System Analysis Toolkit—Non-Proprietary; URL: [www.psat.anl.gov:80/default.html](http://www.psat.anl.gov:80/default.html)) for vehicle designers. This nonproprietary version of Argonne's PSAT software is an accurate, flexible simulation tool to help in developing fuel cell and hybrid-electric vehicles. Simulation is increasingly important in vehicle development because of the large number of possible advanced powertrain configurations. Ford, General Motors, and DaimlerChrysler directed and funded Argonne's development of PSAT-NP through the DOE FreedomCAR partnership (URL: [www.eere.energy.gov/vehiclesandfuels/program\\_areas/freedomcar/index.shtml](http://www.eere.energy.gov/vehiclesandfuels/program_areas/freedomcar/index.shtml)).

Altogether, Argonne has distributed more than 2,000 copies of software to more than 50 commercial and government licensees.

In conjunction with licensing agreements, Argonne often executes R&D agreements aimed at precommercial R&D, through either WFO contracts (as discussed in Supplement 1) or CRADAs. In FY 2003 we executed 30 CRADAs, including amendments to ongoing partnerships. Other types of agreements, such as personnel exchanges and technical service agreements, are used when they meet the needs of the Laboratory and its sponsor or customer.

Some of our recently executed CRADAs had the following objectives:

- **American Plastics Cycle:** Develop new recovery and recycling methods and processes for plastics from scrapped vehicles.

- BP Amoco: Develop a new method of producing acetic acid by anaerobic fermentation.
- CD-adapco: Develop and validate a large eddy simulation model for use in predicting turbulence around fuel bundles in advanced pressurized-water reactors and for integration into adapco's computational fluid dynamics code STAR-CD.
- Chevron Corp.: Develop and evaluate enzyme and biomimetic catalysts for

upgrading heavy crude oil via biological hydrogenation and hydrodesulfurization.

- Flint Hills Scientific: Develop an implantable surface-acoustic-wave micro-sensor for detecting changes in brain states associated with neurological disorders.
- Nanopowder: Contribute to the development of oxide-dispersed nanofluids, a new class of coolants with vastly improved heat transfer properties.

# Supplement 3: Other Tables

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This supplement contains tables characterizing Argonne's activities in the following areas:

- Science and math education
- User facilities

## A. Science and Math Education

Table S3.1 characterizes Argonne's existing educational programs. The total number of appointments and the number of minorities and women are shown for FY 2002 and FY 2003.

## B. User Facilities

Table S3.2 describes experimenters at the Argonne user facilities that have been officially designated as such by DOE. In highly abbreviated terms, these facilities provide the following important scientific capabilities:

- *Advanced Photon Source*. Became operational in 1996, providing superintense x-ray beams meeting research needs in virtually all scientific disciplines and many critical

technology areas; accommodates national research centers in basic energy sciences, advanced synchrotron radiation instrumentation, and structural biology, as well as academic and industrial research teams. (Argonne manages a number of specialized user facilities at the Advanced Photon Source through the Laboratory's scientific divisions.)

- *Intense Pulsed Neutron Source*. Accelerates protons to obtain neutrons, which are particularly valuable for the study of materials through analysis of the motions and structures of atoms.

- *Argonne Tandem-Linac Accelerator System*. Accelerates ions of heavy elements for studies of their reactions, to advance basic understanding of the properties of atoms and atomic nuclei.

- *Electron Microscopy Center*. Provides transmission and scanning electron microscopy for high-spatial-resolution imaging, microanalysis, and *in situ* studies, including studies of *in situ* ion irradiation and implantation effects in metals, semiconductors, and ceramics.

Table S3.1 Participation in Science and Math Educational Programs

Program	FY 2002			FY 2003			FY 2004 Projected Total
	Total	Under- represented Minorities <sup>a</sup>	Women	Total	Under- represented Minorities <sup>a</sup>	Women	
<b>Students</b>							
Instructional Laboratory <sup>b</sup>	3,474	840	1,339	1,550	234	598	2,500
Instructional Vehicle	2,502	1,065	1,289	5,479	1,817	2,197	-
Student Conference	383	-	383	262	-	262	400
Saturday Science Series	-	-	-	78	14	36	-
Science Career Sessions	-	-	-	-	-	-	200
Chicago Workforce Development	-	-	-	23	3	10	25
<b>Teachers</b>							
Argonne Community of Teachers	29	15	23	17	-	10	20
Chemistry Workshop	31	-	22	-	-	-	-
Educational Network Consortium	5,023	-	-	4,721	-	-	4,500
<b>Undergraduate Programs</b>							
Summer Energy Research Participation Program	163	17	57	205	31	63	200
Semester Energy Research Participation Program	34	3	15	26	2	10	25
Community College Initiative	18	8	5	8	4	4	14
Undergraduate Research Symposium	179	-	-	322	-	145	325
<b>Graduate Programs</b>							
Graduate Students — Thesis and Practicum	174	11	55	156	4	34	160
Postdoctoral Fellows	180	10	41	188	10	42	185
National School on Neutron and X-ray Scattering	59	6	21	60	2	13	60
User Programs	817	-	-	976	-	-	1,000
Nanoscience Research Summer School	-	-	-	25	3	9	-
Exotic Beam Summer School	-	-	-	-	-	-	40
<b>Faculty Programs</b>							
Faculty Research Participation	18	3	5	13	2	4	15
Sabbatical Leave	1	1	1	2	-	-	2
Faculty Visits	66	3	13	56	3	12	60

<sup>a</sup> Underrepresented minorities include African-Americans, Hispanics, and Native Americans.

<sup>b</sup> Instructional laboratory numbers include all educational levels and Argonne Information Center participants.

**Table S3.2 Experimenters at Designated Argonne User Facilities — FY 2003**

User Affiliation	Number of Unique Individual Experimenters <sup>a</sup>	Number of Organizations Represented	Percent of Use <sup>b</sup>
<b>Advanced Photon Source</b>			
Argonne	232	1	16
Other DOE Laboratories	136	8	6
Non-DOE U.S. Government	89	13	3
U.S. Universities	1,684	177	52
U.S. Industry	194	48	12
Foreign Government Laboratories	21	25	2
Foreign Universities	262	5	4
Foreign Industry	11	4	2
Other	138	19	3
Total	2,767	300	100
<b>Intense Pulsed Neutron Source<sup>c</sup></b>			
Argonne	42	1	19
Other DOE Laboratories	41	5	18
Non-DOE U.S. Government	-	-	-
U.S. Universities	111	43	48
U.S. Industry	7	6	3
Foreign Government Laboratories	-	-	-
Foreign Universities	28	22	12
Foreign Industry	-	-	-
Other	-	-	-
Total	229	77	100
<b>Argonne Tandem-Linac Accelerator System</b>			
Argonne	38	1	47
Other DOE Laboratories	12	4	6
Non-DOE U.S. Government	1	1	0
U.S. Universities	63	24	22
U.S. Industry	-	-	-
Foreign Government Laboratories	8	4	4
Foreign Universities	57	22	21
Foreign Industry	-	-	-
Other	-	-	-
Total	179	56	100
<b>Electron Microscopy Center</b>			
Argonne	63	1	71
Other DOE Laboratories	-	-	-
Non-DOE U.S. Government	1	1	1
U.S. Universities	22	11	20
U.S. Industry	2	2	2
Foreign Government Laboratories	1	1	1
Foreign Universities	6	6	5
Foreign Industry	-	-	-
Other	-	-	-
Total	95	22	100

<sup>a</sup> Unique individual experimenters are counted only once, even if they travel to the Argonne user facility multiple times during the year.

<sup>b</sup> Percentage of experimental activity or use. Time devoted to maintenance or upgrading of the facility is not included.

<sup>c</sup> For the Intense Pulsed Neutron Source, the percent of use was calculated from the numbers of individual users, not from experimental time.

