The vehicle of the future may have a fuel cell using a microchannel fuel processor under the hood. Pacific Northwest National Laboratory has developed a fuel processor and fuel cell concepts for this application.

The William R. Wiley Environmental Molecular Sciences Laboratory helps educate students and scientists to meet the demanding multidisciplinary challenges of the future. Pictured are University of Washington doctoral students and a Pacific Northwest National Laboratory materials scientist.

Border agents from the Czech Republic recently learned how to use new technologies to detect materials or components of weapons of mass destruction being shipped across borders. One instrument is the Pacific Northwest National Laboratory’s Acoustic Inspection Device (pictured), which identifies contents of sealed containers.

Waste vitrification chemically and thermally converts heavy metals and radioactive elements into a durable, leach-resistant glass. Vitrification technology has been under development at Pacific Northwest National Laboratory for over 25 years. It has been applied to the U.S. Department of Energy's high-level radioactive wastes and to municipal wastes.
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PACIFIC NORTHWEST NATIONAL LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC06-76RL01830

PNNL-14602

This document was printed on recycled paper.
(8/00)
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Foreword:
Director’s Statement
Pacific Northwest National Laboratory—Remarkable Ideas, Remarkable Results

PNL will transform discoveries at the frontiers of science into beneficial solutions for the U.S. Department of Energy (DOE), the nation, and the world.

A World of Opportunity

The 21st century presents significant challenges and opportunities for the world of science and technology (S&T). Growing concerns around energy supplies and distribution, national and homeland security, and the health of our environment require an accelerated pace in creating technology solutions. These solutions are dependent upon fundamental advances in our understanding of complex chemical, physical, and biological processes that govern the behavior of natural and engineered systems at molecular to real-world scales. Delivering such advances anytime in the near future requires transformations in how we conduct both the research and operational sides of science. The successful and timely delivery of scientific discoveries to beneficial applications is key to managing the significant and fast-paced challenges our country and world face. Our contributions will allow our nation to enjoy a strong economy and a safe and reliable energy system, while protecting the environment, ensuring a healthy populace, and stabilizing global threats. This is the core of our vision and the long-term measure of our success.

A New Science

Essential to our vision is our promise to develop a new approach to science that fully integrates the key principles of physical, chemical, and biological sciences to focus on total solutions to big problems. For example, systems biology—the ability to understand and mimic the powerful and selective behavior of life systems at the molecular level—is a fundamentally important scientific frontier because of its potential to create transforming knowledge and solutions. We will infuse our integrated strengths in chemistry, materials, catalysis, and high-performance computing into our biological and environmental science programs to create new methods and investigative tools that will revolutionize the study of living systems. This vision builds upon our proven ability to engage the intellectual, instrumental, and computational capabilities across the Laboratory. We will also engage world-class partners from across the scientific community and industry, becoming the focal point for systems biology capabilities and information. And we will continue to work closely with our customers to rapidly translate new discoveries into deployable solutions.

This approach of closely merging research with final solutions will impact the ways we bring staff together from across the organization, invest in capabilities, engage university and industry partners, improve our research operations, and work in our community. Specifically, we must maintain a research campus that enables us to uphold the vitality and flexibility of the Laboratory to respond to emerging DOE needs; attract, develop, and retain the highest caliber people; and reinforce the S&T vitality of our region, while strengthening our visibility and reputation broadly.
Research Campus of the Future. Upgrading and renewing our core capabilities is critically important to our future. We are placing a high priority on relocating mission-critical capabilities from aging facilities scheduled for closure as part of Hanford cleanup, acquiring a proteomics capability as part of the DOE Genomics:GTL Program, building a bioproducts facility with Washington State University, and embarking on a 10-year plan to maintain state-of-the-art capabilities within the William R. Wiley Environmental Molecular Sciences Laboratory. Our strategy also includes a long-term plan to make certain that we have the resources to add, upgrade, and maintain laboratories, infrastructure, and equipment across the PNNL complex.

Local and regional research and development (R&D) advocacy. We need a vital community to attract and retain staff, and we need a thriving S&T community to realize our vision. To that end, it is important that we emphasize this type of growth in our community and in our region. Strong, multilateral university partnerships are essential to that goal, as are mutually beneficial ties with industry. We will be a catalyst for changing the face of DOE in the region from a focus almost exclusively on environmental cleanup to developing and deploying broadly beneficial S&T.

Integration is the Key to Success

Our strong bias for integration—one of our historic strengths—will distinguish us from other laboratories in several ways. Working closely with our university partners, we will strengthen the integration of chemical, physical, and biological sciences, equipping a new generation of physical-chemical biologists with the methods, tools, and experience to respond to tremendous opportunities in systems biology. With our DOE customers, we will translate methods and ideas from our fundamental science programs into our applied programs and from one DOE mission area to another, advancing discoveries at the interfaces of disciplines and missions. With our industrial partners, we will excel at transforming our S&T results into useful and practical commercial solutions with significant economic benefit to the local community, region, and the world.

Getting Down to the Business of R&D

We continue to emphasize our management philosophy of simultaneous excellence—the delivery of mission-related S&T, enhanced by improvements in research management and operations, and accompanied by strong community citizenship. In recent years, we have developed a strong culture of continual improvement and self-assessment, setting records within the national laboratory system for external certification, and establishing the basis for contract improvements in laboratory oversight and management. Our task now is to couple our strong culture of continual improvement with a renewed emphasis on making our research more productive and impactful. Our new Laboratory contract, through its emphasis on vision and scientific and technical performance, establishes both the expectation and opportunity for success in this regard.

At the end of the day, the ultimate proof of our value lies in the tangible results we deliver. This plan presents the Laboratory’s vision and plans for reaching its full potential for you—as a customer, partner, staff member, or concerned citizen.

“Excitement about science is part of the culture at PNNL. I plan to make sure that type of enthusiasm prevails by fostering a work environment where people get to do what they do best. As part of DOE’s critical science mission, PNNL will continue to be the place where S&T meet, transforming discoveries into tangible, real-world solutions.”
The Value and Structure of This Plan

This Institutional Plan documents our strategy to meet future DOE mission and national needs and achieve our Laboratory vision.

The Value of This Plan

This Institutional Plan describes the most important elements of our five-year plan to meet evolving DOE mission needs and provide outstanding value to the nation. Though this plan specifically focuses on the next five years, it reflects our understanding of what we must be working toward to meet DOE’s and country’s needs for the next several decades.

This is a particularly exciting and crucial time for science. Exciting, because the scientific community is making order-of-magnitude strides in understanding the fundamental building blocks of human biology, creating computational models of increasingly complex natural phenomena, and manipulating matter at the atomic scale. Crucial, because our country is faced with deploying homeland and global security systems to counter ever-changing physical and environmental threats, and developing new energy production and transmission systems to increase the nation’s energy security. We are determined to seize this opportunity, and through this Institutional Plan, have laid the groundwork to meet these challenges head-on.

Institutional Planning is Integral to Laboratory Management

We continually evaluate changes in the many environments (scientific, technical, political, and social) in which we operate, and align our strategy in response to those changes. Producing this plan is an essential step in developing, articulating, and obtaining approval of our strategy.

We work closely with DOE to understand and respond to its needs. DOE’s Strategic Plan and mission strategies give us the context for our highest-level goals and scientific objectives. Through our institutional planning process, we solidify the objectives, measures, and targets that will guide our work during the next several years. The Institutional Plan represents the integrated work plan that we will follow to meet our contract objectives, and it serves as a basis for our annual performance plan with DOE.

The Institutional Plan and our internal Laboratory strategy provide the context and five-year work plan for our internal business plans and allocation of resources. The evolution of these strategic planning documents, and their critical roles in guiding the direction of the Laboratory, are the reasons that the development of this plan and DOE’s approval of it are so important.

Plan Structure Geared Toward Customers

This plan provides the information requested by DOE’s institutional planning guidance, and it fully expresses our strategy for the next five years. In contrast to our previous plans, all information related to our support of DOE’s specific mission areas is consolidated into single chapters, and supporting information is shifted to appendices or referenced to other documents. This Institutional Plan, coupled with
our Performance Evaluation and Measurement Plan, constitutes our first attempt at a five-year S&T work plan. As this is a first attempt, we expect to significantly refine it in future drafts. The content of each plan section is explained below.

- Chapter 1 presents the Laboratory’s strategy, which includes our mission, vision, major objectives and goals, and implementation approach.

- Chapters 2 through 5 describe our support to each of DOE’s missions and programs. For science, energy resources, national security, and environmental quality, we have consolidated all relevant information:
  - Mission roles, strategic intent, and aligned resource projections
  - Articulation of DOE’s current and future needs and our ongoing and anticipated responses, with highlights of our major initiatives
  - Summaries of our Work for Others and their relevance to DOE
  - Infrastructure needs relevant to each mission.

- Chapter 6 states our goals and intentions related to enhancement of research management and our operational improvement agenda.

- Chapter 7 describes our essential efforts in community service and long-term stewardship of the Laboratory.

- The appendices provide required or supporting information.
  - A Partnerships
  - B Pacific Northwest National Laboratory Key Facilities
  - C Pacific Northwest National Laboratory Profile
  - D Resource Projections
  - E Laboratory Directed Research and Development: Renewing the Capabilities at PNNL
  - F Pacific Northwest National Laboratory Organizational Chart

Plan Structured for Ease in Finding Information

The two-page modular format of this plan makes it easier for readers to quickly spot information that is of interest to them.

- By scanning the topics, which also form the table of contents, readers can quickly see the type of information contained in this plan.

- More detail is gained from the thesis statements, which provide the most important point of the module. Readers can then easily decide which modules they want to read.

- The most detail is in the module’s text and figures.
1—Laboratory Strategy
1.0 PNNL's Mission, Vision, and Strategy—An Overview

Our operating principle of simultaneous excellence in S&T, laboratory operations, and community service enables us to deliver on our mission and implement our strategy.

The central focus of our strategy is delivery on our mission. Our Laboratory vision and strategy, respectively, show where we intend to be in the next 20 years and what we will do during the next 5 years to make progress on getting there.

Mission

PNNL performs basic and applied research to deliver energy, environmental, and national security for our nation.

We provide science-based solutions to DOE’s challenges of expanding energy, protecting national security, conducting world-class scientific research, and resolving the environmental legacy of the Cold War. We develop and maintain significant R&D capabilities to create new scientific knowledge. We deliver substantial value to our customers by fully understanding their needs, creating responsive new ideas and capabilities, and delivering exceptional results, which benefit our community, the region, and the nation. We achieve this through our outstanding staff, demonstrated excellence in research management and laboratory operations, and high-value partnerships.

Vision

PNNL will be recognized worldwide and valued regionally for our leadership in rapidly translating discoveries into solutions for major challenges in energy, national security, and the environment by integrating the chemical, physical, and biological sciences.

We intend to advance the reputation of the Laboratory to a degree that the best chemical, physical, and biological scientists from around the globe spend time working here. Increased leadership in professional societies, high-impact publications, hosting visits to the Laboratory by distinguished scientists, and recognition by the scientific community are some of the ways we will measure our progress.

Our regional value is essential to our future, as we help ensure the economic stability of our community and the broader S&T vitality of our region. We will build advocacy among university and industrial partners, resulting in economic and political environments supportive of national R&D agendas. We will gauge our contribution to the region through increased relevance and impact of our university and industrial collaborations, the success of our technology transfer programs, and our ability to attract new R&D companies to the region.


Laboratory Strategy
We will continue to refine and strengthen our historical expertise in integrating science across the various mission disciplines, as well as the integration of science to application. Our success in this area will be measured by the quality, relevance, and impact of our science-based solutions and increased roles in supporting our customers.

**Laboratory Strategy**

To achieve the elements of our vision, we are developing a growth strategy that meets the S&T needs of DOE while ensuring the long-term viability of PNNL and the R&D climate in our region. The top elements of our Laboratory strategy, as illustrated in the figure, reflect the value we provide to DOE.

Our principal value is the delivery of high-quality S&T solutions, which make significant impacts on DOE’s (and the nation’s) most critical challenges in science, energy, national security, and environmental quality. As the Laboratory owner, DOE also values effective and efficient conduct of facility and business operations that support mission delivery, while ensuring the protection of our staff and neighbors and long-term institutional stewardship. These qualities will ensure that we build the capabilities needed to meet the nation’s S&T needs for the next several decades.

We will deliver our Laboratory strategy using Battelle’s operating principle of ensuring simultaneous excellence in all facets of Laboratory management. We are committed to ensuring that our management attention and discretionary resources are properly balanced across delivery of S&T, conducting work operations with excellence, and addressing the needs of communities and the region in which we work.

The three elements of value we deliver to DOE frame the key tenets of our strategy.

- **Mission Delivery and S&T Excellence** – As a multiprogram laboratory, we excel in creating and rapidly translating scientific discoveries into solutions to the greatest challenges faced by all of DOE’s missions. Our program leadership, user facility impacts, and scientific accomplishments are widely recognized.

- **Research Management and Operational Excellence** – Our Laboratory is the most effective and efficient in the DOE system at delivering outstanding research and maintaining excellent operational practices.

- **Community and Stewardship Excellence** – We build and maintain state-of-the-art facilities, valuable regional partnerships, and supportive work environments, which enable our staff to deliver innovative science and substantial benefits to the communities in which we work.

Modules 1.1, 1.2, and 1.3 provide summary information on each of the three strategic objectives and their associated goals. The subsequent chapters of this Institutional Plan align with these objectives and provide the remaining details on what we will accomplish.
1.0.1 Institutional Issues and Planning Assumptions

Effective, multilateral partnerships within and across the DOE offices we serve are essential to our strategy and to successfully achieving our vision.

We Face Three Urgent Challenges

Challenge No. 1 – 300 Area

As one of DOE’s Office of Science (SC) multiprogram laboratories, we provide scientific research capacity and advanced scientific knowledge to support all of DOE’s high-level strategic goals as well as key interagency R&D priorities. Our core capabilities for supporting these goals are outlined in Module 1.1.2 of this document. A significant portion of the facility infrastructure needed to deliver these capabilities resides in a set of aging, Cold War legacy facilities that make up the 300 Area of the Hanford Site. These facilities compose a third of PNNL’s research space and represent the majority of DOE’s laboratory space dedicated to multimission programmatic research. However, they also represent a significant infrastructure liability, including tens of millions of dollars in deferred maintenance, approximately $300 million in decontamination and decommissioning costs, facilities situated over and adjacent to contaminated sites, and facilities poorly configured for future research needs. DOE’s legacy cleanup responsibility encompasses these facilities and plans are under way to accelerate this activity to reduce costs and meet cleanup goals.

As part of an aggressive strategy to address 300 Area transition and reshape our campus, we are evaluating future mission needs and developing a capital asset acquisition plan to provide needed facility capabilities. This will enable us to retain and advance core research capabilities, including unique ultratrace detection, radiochemistry, and biogeochemistry capabilities that are important to DOE’s cleanup, energy, science and weapons nonproliferation missions, as well as to the Department of Homeland Security (DHS), and other agencies. This also provides the opportunity to consolidate and co-locate capabilities to reduce our legacy footprint, increase operational efficiency, and enable research integration for the future.

As a result of the uncertainties associated with 300 Area building availability, the programmatic forecasts presented in this document are based on the assumption that these capabilities are available during this planning period. However, there are considerable management and timing challenges, including the need to balance an aggressive plan to reduce hazards and contain material inventories in preparation for the transition requirements associated with sustaining operating facilities and building future programmatic capabilities. We are currently seeking agreement with and support of this transition strategy from our major customers, following DOE’s capital asset acquisition process, as appropriate.

Challenge No. 2 – Shared Responsibility for the Laboratory

In its leadership role to advance the nation’s S&T capacity, SC closely coordinates the research activities at its multiprogram laboratories to promote the transfer of its basic research results into advances that serve all of DOE’s missions. In this capacity, its laboratories serve a diverse set of science and technology sponsors from across the DOE and other funding organizations. As an SC multiprogram
laboratory, we integrate science to solve significantly challenging problems in energy, national security, and the environment. This ability to bring science to bear on problems is a strength of ours, and is key to realizing our vision; however, it presents a fundamental stewardship challenge.

To continue providing high-impact science and science-based solutions, we must sustain state-of-the-art R&D capabilities. SC has provided exceptional support to meet our upgrade, maintenance, and development requirements; however, delivering the accomplishments outlined in this plan will require significantly increased support. Achieving this support will involve broad partnerships with our major customers to help define and meet mission-driven needs for capability development, research equipment, and research facilities. The 300 Area transition is the most pressing and significant issue we must deal with in the next five years, but it certainly is not the only driver for shared responsibility, which can occur at many levels within the Laboratory’s programs.

We are looking now for a commitment in principle to this concept from our major customers, and will work with SC and appropriate DOE offices on the mechanisms needed to develop a practical and valuable approach for ensuring our continued ability to deliver unique capabilities and solutions to our multiple missions.

Challenge No. 3 – Local and Regional Vitality:
PNNL as an Enduring DOE Asset

This plan presents a picture of S&T growth for the Laboratory. This growth will be fueled by strong leadership within our mission and program priorities and enabled by the successful operation and stewardship of the Laboratory. However, the most critical ingredient for this growth is our staff. A vital community and a vigorous R&D environment are prerequisites to our ability to recruit and retain the numbers and quality of staff we will need to realize our vision.

As the numbers of science and engineering graduates decreases nationally, all R&D organizations are challenged to attract S&T staff. However, PNNL faces another situation that affects our ability to attract talent across the organization. As DOE’s cleanup mission works toward closure at Hanford, labor projections for the local economy over the next 10 to 20 years take a significant downturn. The losses will occur in the community’s high-end jobs, representing a disproportional economic impact and affecting the community’s ability to maintain services and amenities that are attractors to developers and residents. As an increasingly important employer and source of stability in the community, it is critical that the Laboratory help stimulate replacement economic growth. It is also important that we catalyze R&D growth in the region around us. This growth requires higher levels of state support for R&D and will drive an active constituency for federal (including DOE) science programs and budgets. We recognize that stimulating significant growth in DOE and other federal programs consistent with our vision and core capabilities will be a challenge, as will be realizing high-end R&D growth in the region beyond the Laboratory.

To meet these challenges, we are aligning our capability and business investments, and are working closely with our DOE field office, congressional representatives, and industry and university partners in the community and the region. The research and staffing outlook described in this plan assume that these activities successfully maintain a vibrant community and regional R&D environment.
1.1 PNNL’s S&T Excellence is Essential to DOE’s Missions

We will deliver exceptional S&T results that significantly impact DOE’s most important challenges.

In this module we list the most important S&T goals we intend to achieve between now and 2008. Modules 1.1.1 to 1.1.4, respectively, describe the mission drivers, S&T capabilities, current program status, and key accomplishments relevant to our vision.

Science Mission

We will develop PNNL into a world-renowned laboratory for the scientific community, focused on critical challenges in the chemical and environmental sciences, systems biology, and atmospheric sciences and global change (Chapter 2).

Our science mission will provide new tools and state-of-the-art facilities that will be a cornerstone in the nation’s scientific infrastructure, increase the fundamental understanding needed to resolve important scientific questions, and produce discoveries that provide the basis for new, mission-relevant applications. In partnership with other national laboratories and universities, we will:

- Transform how biological systems are described and understood by profoundly impacting how experiments on cellular systems are performed and how the resulting data are analyzed and interpreted.
- Establish a national position and agenda in interfacial chemical catalysis that will significantly enhance our understanding of the physical chemical processes in control of catalytic activity and selectivity.
- Deliver the foundations for the next-generation, physics-based climate models, and create next-generation models for effective climate policy decisions.
- Increase the efficiency of high-performance computing for chemistry, molecular science, biology, regional climate modeling, and subsurface science challenges.
- Optimize our operation of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), with the goal of exceeding the scientific impact promised when EMSL was conceived and built.

Energy Mission

We will expand scientific knowledge and create breakthrough technologies for the energy system of the future, providing secure, clean, affordable energy in a carbon-constrained world (Chapter 3).

We will enhance existing energy systems to improve efficiency, security, and reliability, and to bridge the gap between these systems and tomorrow’s hydrogen economy. By working with DOE and other customers and partners, and building on advancements in systems biology, catalysis, and computation, we will:

- Reduce the dollar-per-kilowatt cost of solid oxide fuel cells by 50 percent.
- Enable existing nuclear plants to safely extend their operating licenses by decades.
- Provide the means to transform agricultural byproducts into high-value chemicals and products, supporting the DOE Office of Energy Efficiency goal to create a $1 billion annual bioproducts business.
- Deliver technologies for producing both electricity and hydrogen from fossil fuel, with carbon sequestration.
Provide new information and energy technologies that will transform today’s energy system into one that is intelligent, robust, reliable, and secure. This comprehensive, intelligent grid of the future can save the nation $80 billion of its projected $450 billion investment in energy infrastructure over the next 20 years.

Advance transportation technology through the development of lightweight materials, fuel cells, and emission management technologies for the automobile of the future.

Apply economically feasible solutions to challenges associated with hydrogen production, storage, distribution, and safety.

National Security Mission

We will be the leader in applying fundamental and applied sciences to create innovative solutions that prevent the proliferation of weapons of mass destruction, ensure compliance with international arms control treaties, and protect the nation’s critical infrastructures (Chapter 4).

PNNL’s programs in national security and homeland defense are built on a strong link between our science programs and our engineering base. We have established four mission areas that align our S&T capabilities with the challenges of our major clients as follows:

- Reduce treaty violations and risks to global security by delivering advanced S&T capability to the design and leadership of U.S. government initiatives targeting the international proliferation of nuclear, chemical, and biological weapons.
- Apply advances in S&T to deliver robust detection, analysis, and decision systems that protect national assets, preclude strategic surprise, and defend against attacks on the U.S. homeland.
- Become the provider of choice for information and analytical technology products serving the U.S. intelligence community.
- Provide innovative technology solutions and leadership to facilitate transformation of the military for the 21st century.

Environmental Mission

We will be the leading S&T laboratory for expedited cleanup and sustainable processes (Chapter 5).

We will continue to provide science-based solutions to DOE’s most critical national cleanup challenges and will expand the application of our capabilities to other national and international environmental challenges. We will:

- Substantially reduce the cost, time, and risks associated with restoring the environment affected by the legacy wastes from the nation’s nuclear weapons production program.
- Protect ecological and human health by ensuring the safety of the workers performing cleanup activities as well as protecting the public and environment adjacent to cleanup sites.
- Generate the discoveries and develop the technologies that will help sustain the global environment through improved management of ecosystems, carbon generated from energy and other sources, and water resources.
- Provide scientific information that supports decisions around establishment of the Yucca Mountain repository.
1.1.1 Relevant DOE Mission Drivers and S&T Strategy

Our S&T goals in Module 1.1 and our programs in Chapters 2 through 5 are responsive to DOE's Strategic Plan.

DOE Mission and Program Priorities

DOE's science strategic goal is to provide world-class scientific research capacity needed to ensure the success of DOE missions in national and energy security; to advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences; and to provide world-class research facilities for the nation's science enterprise. Our programs are aligned with four out of the eight strategies that DOE has set for its science programs:

1. Advance energy-related biological and environmental research, building foundations in genomic science, climate modeling, contamination and transport modeling, and related interdisciplinary sciences (Modules 2.2.1–2.2.3). The work we will do in support of the Office of Biological and Environmental Research (BER) on this strategy, including the developments that will occur in the DOE Genomics: GTL High-Throughput Proteomics facility that we hope to secure at the Laboratory, will be beneficial to DOE's science strategy regarding development of new diagnostic and therapeutic tools and technologies for disease diagnosis and treatment, noninvasive medical imaging, and biomedical engineering (Module 2.5).

2. Advance nanoscale science built around foundations in materials, chemistry, engineering, geoscience, and energy biosciences, leading to improved energy technologies and systems (Modules 2.3–2.3.1).

3. Advance scientific simulation and computation by applying new approaches, algorithms, and software and hardware combinations to the critical science challenges of the future.

4. Provide or support access by the nation's scientific community to world-class, computational and networking facilities that support advancements in practically every field of science (Modules 2.4–2.4.1).

DOE's energy strategic goal is to protect our national and economic security by reducing imports and promoting a diverse supply of reliable, affordable, and environmentally sound energy. This overarching intention has two subgoals: reduce dependence on energy imports and develop new energy technologies. Our programs are aligned with 7 of 14 strategies supporting these goals:

1. Collaborate with industry to develop the FreedomCAR, a demonstration of zero-emission, hydrogen-fueled, fuel-cell-powered vehicle (Module 3.1.2).

2. Develop and bring to market technologies that advance energy efficiency, including waste heat recovery and solid-state lighting (Module 3.1.4).

3. Ensure the availability of nuclear fuel to meet potential supply disruptions (Modules 3.5–3.5.1).

4. Accelerate the shift toward the hydrogen economy by developing and improving technologies to produce hydrogen using renewable energy, nuclear energy, and fossil fuels while overcoming obstacles to hydrogen storage and distribution (Modules 3.1.1 and 3.3–3.3.1).
5. Conduct R&D programs that displace or sequester carbon and reduce emissions (Module 3.4).

6. Research renewable energy technologies and work with the private sector in developing these domestic resources (Modules 3.1.3–3.1.3.1).

7. Develop technologies to reduce the vulnerability and increase the reliability of the electricity supplies, focusing on superconducting materials and distributed generation, relatively small-scale and modular energy generation devices (Modules 3.2–3.2.1).

DOE’s defense strategic goal is to protect our national security by applying advanced science and nuclear technology to the nation’s defense. Within this overarching goal are three subgoals, one of which focuses on nuclear nonproliferation. PNNL’s programs, including our work for others, are aligned with all five of the strategies that will be implemented to address the nuclear nonproliferation goal (Modules 4.1–4.1.6 and Module 4.2):

1. Prevent the spread of materials, technology, and expertise relating to weapons of mass destruction.

2. Eliminate or secure inventories of surplus materials usable for nuclear weapons, and redirect excess foreign weapons expertise to civilian enterprises.

3. Secure radioactive sources that pose the greatest threat as potential ingredients in Radiological Dispersal Devices, or dirty bombs.

4. Enhance our ability to detect weapons of mass destruction, including nuclear, chemical, and biological systems.

5. Work to reduce the risk of accidents in nuclear facilities worldwide by improving safety regimes in Russia and other countries.

In addition, we are aligning our capabilities with the priorities of the intelligence community’s need for analytical technologies (Module 4.4), DHS’s need for advances in S&T for next-generation tools (Module 4.5–4.5.1), and the Department of Defense’s (DoD’s) goal to transform the military for the 21st century (Module 4.6.1).

DOE’s environmental strategic goal is to protect the environment by providing a responsible resolution to the environmental legacy of the Cold War and by providing for permanent disposal of the nation’s high-level radioactive waste. PNNL is supporting the following strategies for these goals primarily by providing S&T to Office of Environmental Management contractors:

- Review the remaining risks in concert with regulators and stakeholders to determine the most appropriate remediation schedules and approaches (Module 5.3).
- Focus S&T to directly address specific, applied technology needs for cleanup and closure for the next 5 to 10 years (Modules 5.1–5.1.5 and 5.4).
- Establish a permanent geologic repository for high-level waste and spent nuclear fuel at the Yucca Mountain, Nevada, site (Module 5.2).
- Investigate advanced technology options to promote future waste-management alternatives, which could significantly reduce the amount of future, spent nuclear fuel requiring disposal (Module 5.2).

In addition, we are aligning the capabilities that have been developed largely in response to DOE’s legacy waste management mission to anticipate and address future mission needs that require a fundamental understanding of complex environmental systems to protect and sustain global environmental security, environmental and public health, and the economy.
1.1.2 S&T Capabilities

Our plan for substantial S&T accomplishment requires that we sustain existing core technical capabilities, create new capabilities, and house them all in a productive modern research campus.

Our strong base of established core technical capabilities, listed below, is well aligned with our current set of programs and many of our customers' future needs. Appendix B provides summary descriptions of research facilities and equipment that are part of these capabilities.

- **Chemical science and engineering** - trace and complex analyses, including instrument design; molecular modeling, including structures; radiochemistry; interfacial catalysis and advanced separations; micro chemical and thermal systems; chemical and biochemical process design and control

- **Material science and engineering** - macro- and nano-scale synthesis; materials manufacturing; environmental and radiation degradation; glass and high-temperature oxide (fuel cell) performance

- **Biological science and biotechnology** - microbial systems; analyses and modeling of biomolecules and systems; biological effects of radiation and chemicals; dosimetry

- **Computational science and information technology** - large-scale data management; problem-solving environments; high-performance computing in molecular sciences; computer system design and security; information analytics and visualization

- **Nuclear science and technology** - trace detection and analysis; reactor safety; fuel cycle processes and related security systems; nuclear-based detectors; non-destructive evaluation

- **Environmental sciences and engineering** - atmospheric measurement and remote sensing; climate modeling; geo- and biogeochemistry; fate and transport of contaminants; ecological monitoring, management, and remediation; integrated assessments and policy

- **Engineering of integrated systems** - device and system design and control; diagnostics and prognostics; robotics; systems engineering and assessments; integrated security systems; energy codes and standards.

Though individual disciplines or capability areas are listed, we recognize that our most important innovations come from working at the interfaces among the major capabilities. In addition, we enhance our capabilities through strategic partnerships with universities, other national laboratories, and industry.

**Investments to Enhance Our Capabilities**

We enhance capabilities through funded R&D programs, direct DOE investment (e.g., budget line items), recruitment, and investment of internal PNNL and Battelle overhead funds. Substantial ongoing investment is required to maintain and enhance existing capabilities and create new ones to respond to future DOE needs. The drivers for making changes in capabilities (either divestment or enhancement) include the rapid pace of discovery and innovations in scientific equipment, changing customer needs, and new facility and infrastructure plans at the Hanford Site. With respect to our supporting research infrastructure, our long-term strategies for information technology and facilities are described in Modules 6.3 and 7.3, respectively.

To develop new ideas and technical capabilities to meet future program needs, we leverage program funds and make internal overhead investments, principally through
Laboratory-level initiatives and our Laboratory Directed Research and Development (LDRD) Program. We use a life-cycle approach to manage our initiatives. The figure shows the four stages:

1. Understand DOE’s needs and our potential roles in meeting them.
2. Develop the new ideas, staff, and infrastructure that are needed to respond.
3. Work with DOE to build programs that leverage these capabilities.
4. Establish enduring, major programs with DOE and our other customers, which are able to produce deployable, science-based solutions.

Following is a list of our current Laboratory-level initiatives, including the modules that contain details on each initiative. Details on our LDRD and peer review processes that support these initiatives are found in Appendix E.

- **Biomolecular Systems** (Module 2.2.1.1) – Build multidisciplinary, collaborative research programs that integrate molecular biology, biochemistry, physics, and computational science in ways that allow us to understand complex biological systems critical to DOE mission needs.

- **Nanoscience and Technology** (Module 2.3.1) – Establish foundational capabilities that enable us to contribute to key areas of nanoscience and to apply nanotechnology to needs in catalysis and biodetection.

- **Computational Science and Engineering** (Module 2.4.1) – Enhance computational science capabilities for creating multidisciplinary, computational approaches to solve complex DOE problems, create high-performance software suites, and make major advances in computational science.

- **Bio-Based Products** (Module 3.1.3.1) – Enhance capabilities that can provide DOE with innovative technologies to cost-effectively convert biomass into high-value products.

- **Energy Systems Transformation** (Module 3.2.1) – Provide new information and energy technologies that will transform the nation’s energy system, from all fuel sources to domestic and industrial end uses, into a market-driven grid system, which is intelligent, efficient, reliable, and secure.

- **Carbon Management** (Module 3.4) – Provide the tools and understanding that can shape the nation’s approach to addressing climate change and the capabilities needed to provide science-based solutions such as subsurface carbon sequestration.

- **Homeland Security** (Module 4.5.1) – Create major advancements in the fusion, analysis, and visualization of massive information sources and in robust, low-cost systems for collecting, concentrating, and sensing chemical, nuclear, and biological weapons to improve homeland security.
1.1.3 Program Status and Summary Resource Projections

Growth in our programs reflects the substantial benefits received and expected by our customers, and it will provide the additional resources essential to achieving our Laboratory strategy.

Resource Projection Story

The resource level we project is an important indicator of how much our customers value our programs. The first figure shows a steady increase in our customers’ investment in our staff, facilities, and programs. Our DOE programs are staying steady or growing in response to changing needs. We are providing substantial support to the DHS in response to the significantly increased terrorist threats against the U.S. homeland. (Current DHS funding in the range of $25 million to $35 million per year supports PNNL staff, and the balance is going to a large, multiyear project for establishing weapons detection systems at U.S. border crossings.) Our Work for Others (WFO) funding reflects the increasing value we deliver to other governmental agencies and is remaining at a manageable level. The second figure shows a modest but steady increase in staff deployed to our R&D programs, while our nondirect staffing level declines slightly, reflecting improved research productivity.

Our projections are conservative to ensure that our plans and investments can be delivered with a high degree of certainty. However, we believe that the significant and increasing challenges being faced by our customers can lead to additional programmatic growth over this time period. This growth is important because it provides additional internal resources that will accelerate our progress toward our vision. In particular, we believe there are significant opportunities for further programmatic investment in biological and environmental research, energy technologies that support administration priorities, and national and homeland security programs.

Planning Assumptions Around Federal Budgets and Policies

Our resource projections are influenced by the direction of federal budgets and policies. We assume that DOE’s overarching mission of protecting national and economic security with advanced S&T will result in continued support for creating world-class scientific research capacity, advanced energy technologies, national security research and applications, and continued environmental cleanup. We believe that federal S&T budgets, including DOE R&D funding, should at least be stable and will likely increase, perhaps substantially, during the next five years.

This view is based on increasing recognition by the Administration and Congress that investments in R&D underpin U.S. technological leadership, stimulate growth in the national economy, increase energy security, and provide solutions for the war against terrorism. We anticipate increased funding for advances in biological, chemical, and physical sciences; energy R&D; and homeland and national security-related programs. We expect funding for environmental R&D to continue to decline as a reflection of the progress being made in DOE’s cleanup programs.
Even if optimistic projections prove accurate, the environment for allocating resources will be highly competitive, with many state governments seeking to support their research universities and attract other research investment as a means to sustain economic growth. The Office of Management and Budget guidelines for making federal investment decisions in basic and applied R&D will drive priorities in budget decisions and shape the evaluation of research programs at DOE and other agencies. DOE and the national laboratories will remain under pressure to improve management practices and to increase research productivity.

How We Develop and Present Our Data

We prepare detailed plans based on the strategy and program direction articulated in this Institutional Plan. An important step in preparing these plans is projecting the funding and staff levels envisioned during the next five years. These projections are essential for preparing investment strategies that will ensure that we have the infrastructure and capabilities needed to support DOE missions. We use standard assumptions for our projections in the Laboratory Funding Summary figure and table. R&D support to Hanford Site programs is included in the resource projections of various funding programs. R&D support to other DOE sites is included in “DOE Site Transfers and Cash Work.” The resource figures for FY 2002 and FY 2003 are actual values.

The Laboratory Funding Summary shows the levels of actual budget authority for the past fiscal year, current year projections based on formal notifications, and future expectations based on proposal and customer interactions. However, it does not include proposed construction line item funding for replacement general purpose facilities.

The Laboratory Personnel Summary shows the levels of Laboratory personnel in Full-Time Equivalents (FTE) for the past fiscal year, current year projections based on formal notifications, and future expectations based on proposal and customer interactions. These values are based on standard assumptions including one FTE equals 1832 work hours per year.
1.1.4 A Record of Accomplishments

PNL will play a major, demonstrable role in advancing DOE’s reputation for delivering science-based solutions for energy, national security, and environmental challenges.

As highlighted below, our historical bias is to drive scientific advances and discovery into new approaches for solving our customers’ challenges and into information that is useful to policymakers. We will continue to seek ways to apply the practical benefit of the science we conduct into all our mission programs.

Systems Biology

As a major but relatively new research thrust at PNNL, systems biology has already made significant impacts in various DOE programs. Systems biology focuses on how different parts of biological systems interact—from the molecular level to the whole organism level—to provide a comprehensive, quantitative, and predictive understanding of cell and organism function.

Because of our special expertise in high-throughput proteomics and microbial systems, we are a key contributor to the DOE Genomics:GTL Program. Staff who are developing that science base are engaging actively with staff who understand the challenges to effective solutions for cleanup, climate change, and biowarfare countermeasures and who appreciate how a better understanding of systems biology can solve those challenges. In environmental research, we are applying systems biology approaches to understand carbon sequestration, which plays an important role in global climate change. In environmental cleanup, we successfully provided comprehensive proteomics coverage of Deinococcus radiodurans, the most radiation-resistant organism known. We are also building projects into our Homeland Security Initiative that recognize the potential application of proteomics to the characterization of biological agents that might signal a threat to homeland security.

Our systems biology program is also leading to biotechnology R&D. We recently reported a breakthrough in single-chain antibody generation; subsequently, our new “library” contains over $10^9$ distinct types of antibodies. It is now possible to create affinity-probes suitable for detecting pathogens and cancer-associated proteins at a speed far exceeding that of any previous technique.

Climate Change

For more than a decade, we have played a key role in implementing the DOE’s Atmospheric Radiation Measurement (ARM) Program. ARM is specifically focused on the impact of clouds on the energy balance of the climate system, which remains one of the most important uncertainties in predicting the extent of climate change impacts.

ARM’s land-based cloud observation systems allow scientists to improve models against observations for more precise climate simulations and weather predictions. This program has turned pioneering remote-sensing systems from intensively manned devices into routine, semiautonomous instruments. ARM observatories are now an integral component of international collaborations and U.S. government research programs sponsored by agencies such as the National Aeronautic and Space Administration (NASA) and the National Oceanic and Atmospheric Administration.

PNNL is also an internationally recognized leader in climate modeling and impact assessment at the regional scale. Our team of interdisciplinary scientists has developed regional scale projections of future climate change and examined its impacts.
on water resources in the western United States between 2040 and 2060. These studies provide the scientific basis for showing how climate change might affect the United States and for developing energy-policy strategies to minimize its adverse effects.

**Information Visualization**

PNNL scientists developed a broad suite of technologies based on “data signature” visual analytics. This signature is derived from relationships within text, science, image, video, etc., with no prior knowledge of the content or structure, that scales to large information spaces. The underlying interdisciplinary science is the creation of these data signatures, the mapping of these into high-dimensional mathematical spaces, the identification of core concepts and themes, and then the visual and highly interactive paradigms. These high-dimensional relationships are projected into visual interaction paradigms closely modeled after the dynamics of the human mind that enable users to discover the unexpected in large, complex data sets.

This technology was recognized as an outstanding contribution from PNNL by the senior leadership of the U.S. intelligence community in FY 2003, along with two of our PNNL staff on assignment to the intelligence community and responsible for successful insertion of this technology into an operating environment. Recent inventions are now included as part of the core suite of technologies within the President’s Terrorist Threat Integration Center and DHS. In addition, two commercial spinout companies have been created around this technology. Major commercial companies, such as Dow Chemical Co., have stated this technology has saved them millions of dollars. These technologies are also being applied within our Systems Biology Program to help manage the vast databases that are being generated as a result of our high-throughput proteomics research.

**Fuel Cells**

To support the nation’s need for a more environmentally sustainable, efficient, and cost-competitive energy future, our fuel cell technologies apply to a wide range of uses, including distributed power for residential, commercial, and utility power plants, as well as for transportation and power for military operations. Building on 15 years of research in material properties, chemistry, and ceramic processing for fuel cells, our team of scientists is now focused on designing, modeling, and fabricating complete fuel cells systems, particularly solid oxide fuel cells. Our extensive modeling and simulation capabilities are helping to optimize individual fuel cells and fuel cell stack materials, and answer questions about the flow and thermal distribution within fuel cell stacks. In 1999, we teamed with DOE Office of Fossil Energy and its National Energy Technology Laboratory to form the Solid State Energy Conversion Alliance, which includes government agencies, commercial developers, universities, and national laboratories, with a common goal to commercialize solid oxide fuel cells within 10 years.

**Use of Catalysis in Treating Engine Exhausts**

With our industry partners we developed an engine exhaust aftertreatment system that converts harmful oxides of nitrogen and particulate matter from vehicle engines into components of clean air. This system uses a nonthermal, plasma-assisted catalysis method to address industry’s need for a technology to meet upcoming exhaust regulations for diesel engines. We transferred this technology to Delphi Corp., Caterpillar Inc., and the Low Emissions Partnership of USCAR. These technology advancements address a roadblock to widespread use of engines that could greatly increase fuel efficiency in vehicles, while reducing the nation’s dependence on foreign oil and the amount of greenhouse gas emitted to the atmosphere.
1.2 Research Management and Operations: Continued Excellence, Improved Productivity

Our continued focus on excellence in research management and operations will ensure protection of DOE assets and will lead to a highly productive research enterprise.

Integrated Management of Research and Operations

We are successfully implementing an integrated management approach to the Laboratory’s principal research and operations functions. By breaking down traditional operational stovepipes, we provide operational management systems that seamlessly work together to protect our staff, the public, and the environment; ensure compliance with all applicable requirements; reduce operational overhead costs; and support conduct of research that produces the outstanding results demanded by our customers. Examples of our outstanding record of operational accomplishment over the last several years are described below.

- We have received outstanding ratings on our Laboratory operations indicators over the last five years.
- We have reduced overhead rates by 20 percent since FY 1994, allowing us to increase the percentage of Laboratory funding directed toward research and investments in scientific initiatives, staff, and facilities.
- We have received and are maintaining the highly respected external certifications for Integrated Safety Management, Voluntary Protection Program, and International Organization for Standardization’s Environmental Management Standard—ISO 14001.

We believe that we are on track to maintain this record of accomplishment through continued vigilance, revitalized approaches that keep staff engaged in operational outcomes, and efforts to ensure increased effectiveness and efficiency. With this strong foundation in place, we will invest in operations and new research processes to increase our research productivity. We believe that the cost of doing this will more than be repaid by the value received by our customers and the progress we will make in achieving our vision.

Defining and Measuring Research Productivity

To support this effort, which we expect to continue over the period of this plan, we have defined research productivity. As a starting point, research productivity refers to both the amount of new S&T created per customer dollar, and the impact or value of the new S&T in terms of 1) solving customers’ most critical challenges, or 2) breakthrough discoveries that are broadly applicable and important S&T innovations. This definition may evolve over time, based on discussions with other laboratories and interactions with DOE Headquarters staff who are responding to the President’s Management Agenda.
Our aspiration is to conceive and build the first-ever national laboratory system of quantitative and qualitative measures and associated measurement processes and tools, which are needed to identify the means to improve research productivity. Some of the measures we are considering include contribution to DOE and other client missions; peer-reviewed publications in the most important journals; numbers of citations, honors, and awards; intellectual property generated; and contributions to the supply of the future S&T workforce and to S&T literacy. We will test and refine this approach until we see substantial progress.

**Improving Research Productivity**

Many variables can have an impact on research productivity, including staff knowledge, skills, and development opportunities; new facilities and equipment; investments in developing new ideas; the number and nature of collaborations and partnerships, both with individuals and with institutions; improved operational processes; and management and administrative support, including help with proposals and publications.

We have selected what we believe are the three major drivers to simultaneously ensure managerial and operational excellence and improve research productivity. These drivers are summarized below and explained in detail in Chapter 6.

- **Leverage our current outstanding operational performance to develop even more effective and efficient practices and tools that deliver scientific, technical, and economically valuable results to DOE and the nation, while simultaneously:**
  - Protecting the health and safety of workers, the public, and the environment.
  - Safeguarding DOE’s assets at PNNL.
  - Increasing funds available for Laboratory renewal.

- **Build and retain a workforce of fully engaged managers and staff** with a mindset for continued operational excellence, the ability to substantially contribute to DOE and Laboratory outcomes, and a clear focus on scientific productivity.

- **Optimize our core research management and work processes for understanding our customers’ needs, integrating multiple disciplines to rapidly develop and deploy high-value solutions critical to DOE’s missions, and enhancing DOE’s assets at PNNL. We will enable and increase the impact of these new processes with a high-performance information management system.**

(a) Engaged staff are fully cognizant of their roles within the Laboratory strategy, are actively developing their skills, and are fully empowered to deliver high-quality work.
1.3 Establishing PNNL as an Enduring Regional Asset

We must sustain a modern research campus and significant, lasting, and mutually beneficial relationships with our community, state, and region to achieve our vision.

Ensuring Long-Term Viability

Over the next several decades we must be able to upgrade the human resources, equipment, and facilities needed to support DOE’s important and increasingly complex research needs. One of the most important factors in doing this is a surrounding region that can provide strong economic and community support to the Laboratory and to national research agendas.

During the next two decades, most cleanup work at the Hanford Site will be completed, potentially reducing employment and the substantial economic benefit it provides to the Tri-Cities. By replacing a significant portion of these jobs, the Tri-Cities and PNNL will be competitive in retaining and attracting the best technical and operations staff. PNNL, DOE, and regional leaders are working together to diversify and grow a substantial R&D business as well as other businesses in the Tri-Cities. This means that community programs and economic development are no longer discretionary, but are strategic imperatives for PNNL and DOE.

Likewise, PNNL and DOE must also make federal and arrange third-party investments to reinvigorate and maintain the Laboratory’s research campus. Finding solutions to DOE’s future challenges and the future scientists and engineers engaged in finding those solutions will require state-of-the-art research facilities and equipment. The region can also play a key role in this by direct investment in the Laboratory’s infrastructure by advocating sustained federal investment in the region.

The Plan

Based on current Hanford Site plans, we are a logical and promising candidate to become a primary source of economic stability in the Tri-Cities. As the most significant federal R&D organization in the Northwest, our research results, coupled with state-of-the-art facilities and equipment, can firmly establish the Laboratory as a long-term, highly valued regional asset. Thus established, we expect to continue to grow and add jobs, attract new R&D organizations to the community, and be seen by private and public entities in the region as a valuable asset worthy of support and investment. Additionally, regional support of DOE’s research agendas not only helps sustain the needed programmatic support at PNNL, but provides DOE’s programs with badly needed budget supplements. If over the next 10 years the Laboratory can realize growth sufficient to support 5000 plus staff, and if 2000 to 3000 new research jobs are created by others to take advantage of our resources, the economic base for the community will be significantly strengthened. Coupling this with the Laboratory’s ongoing community support through financial and volunteer contributions, our ability to attract and more easily retain high-caliber researchers and other staff should be significantly enhanced.
Building and Sustaining Our Research Campus of the Future

In partnership with DOE and the region, we will create and sustain modern research facilities that will attract and keep the best staff and scientific users and support increased research productivity. We intend to pursue the following strategies:

- Clearly describe DOE’s future needs for mission-critical research facilities and equipment and staff capabilities.
- Work with DOE, DHS, and other key clients to obtain funding to build and sustain research facilities.
- Work with regional entities to obtain state and commercial investment to build supporting R&D facilities, such as offices, shops, dry laboratories, and computer space.
- Commercialize DOE-developed technologies to create income streams that can be reinvested in facilities and equipment.
- Enhance the Laboratory’s access to other research facilities and equipment through strategic partnerships with regional universities and research firms.
- Maintain Battelle investment in the Laboratory’s research infrastructure.

Creating Income for Reinvestment in the Laboratory

We are developing technologies that provide high value to our customers, society, and the economy. However, to realize the greatest benefit from these technologies we will use our “best-in-class” technology commercialization program to get them into broad markets. These deployments will also result in income back to the Laboratory, which can be invested in the Laboratory’s staff and infrastructure. These commercialization efforts also provide positive impacts to local and regional economic development. In the next five years, we will focus on:

- Creating significant and increasing cash and noncash value from DOE-derived technologies.
- Creating intellectual property to build a pipeline for commercialization, thus enhancing the relevance of our results and value to the taxpayer by placing them in the marketplace.

R&D Advocacy Through Strategic Partnerships

We are using and establishing strategic partnerships with key regional universities and industries. These partnerships allow us to leverage joint investments and collaborations that help build and sustain our critical research capabilities, while helping build the broad advocacy needed to support the Laboratory as an integral part of our community and region. We will achieve these goals in the following ways:

- Through strategic university partnerships, our science and engineering education programs will help reform and diversify educational programs to produce the next generation of scientists and engineers.
- Through continued investments and volunteerism efforts, we will improve the quality of life and business climate in our community.
- By establishing research capabilities that benefit the region’s research enterprise.

PNL’s strategic investments, corporate contributions, and volunteerism are building broad advocacy needed to create and sustain modern research facilities and enhance the quality of life in the surrounding community.
1.4 Managing a High-Performance Laboratory

We are applying proven private-sector management techniques to the delivery of research, resulting in an effective alignment of resources to achieve our vision.

Our Accountability Model

We are implementing an accountability model adapted from a private-sector model for management, which aligns the governance, management, and performance functions within the Laboratory. The governance function provides senior management attention on the strategic future of the Laboratory. It is accountable to DOE, our other customers, and Battelle to set direction, goals, and strategy, as well as the acceptable levels of performance that management is expected to deliver. Management is accountable for translating goals into tactical objectives and deploying resources to attain those objectives while managing performance within the limits set by governance. The performance level, where the work of the Laboratory gets done, is accountable to management for performing work within the established procedures and guidelines, with attention to minimizing risk.

Governance Sets Strategic Direction

Governance, consisting of the Laboratory Director and senior management, sets the direction of the Laboratory, aligns resource allocations with goals, approves operational and business boundaries, and monitors progress toward goals. Using knowledge of our customers’ strategies and data and information on our past performance, current capabilities, and corporate obligations, the senior managers determine the goals to be achieved and the strategies to employ. They set operational expectations to provide management and staff clear operating boundaries. This step will eventually include establishment of risk boundaries for key operations. They allocate resources to ensure achievement of our goals and management of associated risks. Finally, they monitor performance relative to goals and changes in the business environment, and they adjust budgets and guidance as needed to respond to significant changes.

Management Translates Strategy into Tactics

Management translates goals into tactical objectives, deploys resources to achieve the objectives and manage within risk limits, and provides feedback to governance on performance. Our mid-level managers (management systems, customer relationships, technical staff, and product delivery) perform this management function. With leadership direction on the Laboratory strategy, they develop tactical objectives within organizational business plans to align resources to goals. After governance approval, management deploys resources to execute the business plans, and monitors performance, providing feedback to governance on a regular basis.
In our **Accountability Model**, we ensure performance through communication of strategy and expectations throughout the Laboratory, setting of clear management accountabilities, managed delivery of high-quality products and services to customers, and use of processes that ensure that work is being managed within established risk boundaries.

**Staff Do the Laboratory’s Work**

Supervisors and staff use processes, procedures, and tools to perform day-to-day project activities to accomplish our tactical objectives, while managing within established operational limits. Performance data and trends relative to the goals and objectives are gathered from this level through the use of self-assessment, and are summarized for management and governance to provide information essential for decision-making.

**Assurance Processes Validate Performance Assessments**

Governance and management employ means such as internal audit, independent oversight, peer reviews, and external certifications to provide reasonable assurance that goals are being achieved within approved operational boundaries. We use self-assessment to provide information on performance, and to validate that management systems are performing effectively and efficiently and that accurate and reliable data is being delivered to decision-makers and regulators. Assurance is also used to validate that our customers are being served through our relationship, product delivery, and technical capability management processes with high-quality products and services. (Additional information is provided on peer review in Appendix E.)
1.4.1 The Relevance and Quality of Our S&T Programs

We choose our S&T programs to work on the issues that really matter to DOE and the nation.

Our customers expect us to deliver high-quality, science-based solutions that are directly relevant to their needs. We ensure this by embedding proven research management and operational approaches within our programs and research activities, and by how we operate our facilities. Because these elements are fundamental to the value we deliver, they serve as the primary basis of the Performance Evaluation and Measurement Plan with DOE.

Relevance is Essential

The R&D we perform for DOE and our other customers must be relevant to the challenges they are addressing.\(^{(a)}\) We ensure the relevance of our work by verifying that it meets three criteria:

1. **Program alignment** - We produce the S&T understanding and leadership needed to support the creation of new R&D programs that address emerging DOE challenges.

2. **Value and impact** - The work we perform results in substantial value to DOE, and often to the nation broadly.

3. **Utilization** - The science-based solutions we provide are adopted by other researchers or used by industry in commercial applications. We do this principally through strategic partnerships.

Quality Counts!

Because of the central role the national laboratories play in the nation’s R&D enterprise and the critical nature of challenges being addressed, quality must be a hallmark of our S&T programs. The aspects of quality we focus on delivering are:

- **Creation and innovation** - Using the insights from our application programs, we develop high-potential areas of scientific inquiry. We focus multidisciplinary teams on developing original advances in science and creative technological innovations.

- **Importance** - We ensure that our science outcomes make important contributions to key scientific fields, and our technologies represent substantial contributions to the nation’s technology base.

- **Recognition by others** - We actively pursue recognition of our science-based solutions by others to broaden their use, increase our ability to engage scientific leaders, and enhance DOE’s reputation for delivering science-based solutions.

\(^{(a)}\) This concept is also being strongly emphasized by the Office of Management and Budget in their implementation of the Performance Assessment Rating Tool across all executive departments.
Research Management and Program Leadership

We ensure the relevance and quality of our results, and we increase our research productivity by how we manage and lead our research programs. Our program managers focus on these principles:

- **Leading and partnering** - The complexity of the challenges we address require scientific leadership and the application of resources from other national laboratories, universities, and industry. Cooperative agreements and staff interactions allow us to leverage the best possible resources in carrying out our programs.

- **Science to applications** - The urgency in addressing many national needs requires us to accelerate the translation of scientific discovery to final applications.

- **Research productivity** - In response to the President's Management Agenda and increasing competition for R&D funding, we are improving our operational and research work processes to increase research productivity.

- **Strong project execution** - We thoroughly plan our R&D projects to ensure that multidisciplinary and multorganizational teams properly understand and manage risk. We subject critical project plans to internal and sometimes external peer reviews to ensure their adequacy, and we provide a suite of project control tools to ensure proper execution of all projects.

Value of Research Facilities

Essential requirements for breakthrough science are state-of-the-art facilities and capabilities and supportive management systems. Our focus around enabling quality through operation of research facilities includes:

- **Outstanding staff** - The ultimate source of all our research accomplishments is our staff. We actively recruit, develop, and retain the best possible staff to support current and future Laboratory programs.

- **Research campus of the future** - We are creating a research campus of the future with leading-edge facilities and equipment to address the increasingly complex challenges of our customers and to accommodate the proposed changes in the Hanford Site research infrastructure.

- **Facility value to external users** - A central tenet of DOE’s strategy is to provide world-class research facilities for the U.S. research enterprise. We are providing innovative operational and programmatic means for external scientists to add substantial value to their research by their use of EMSL and our other research facilities.

- **Safe, secure, and reliable operations** - Through our operating principle of simultaneous excellence, we ensure that adequate resources are provided to implement seamless management systems that protect our staff and DOE assets and to ensure that R&D resources are available for use to the maximum extent possible.
2—Science
2.0 Fundamental Science Research

PNL’s fundamental science research is making significant contributions to some of the most difficult and important science issues of our time by integrating our science disciplines, expanding our signature capabilities, and collaborating with the best scientists in the world.

Our intent is to create new science, new understanding, and enduring national assets around our facilities and scientific staff. The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is one such asset; we will strengthen EMSL by focusing its user program on the scientific Grand Challenges of biogeochemistry and biology with broad extramural collaboration. In the future, we plan to develop Grand Challenges in other areas, including complex interfacial catalysis. The outcomes of this research will advance fundamental understanding in each of these fields and speed application into the programs supporting the applied missions of DOE.

Our science strategy requires an approach dependent on integration across classic disciplinary boundaries. The technical goals associated with our vision are ambitious and aligned with the principal initiatives and programs of the DOE’s Office of Science (SC). As described below, they are also aligned with our strengths.

Systems Biology

As the most conspicuous element of our science strategy, we are developing a rapidly growing signature at the intersection of biology, physics, chemistry, and computing. We will place particular emphasis on environmental microbiology and the application and integration of high-throughput analytical and computational technologies at a large scale. This is the key to advancing the understanding of biology at the systems level.

In developing our leadership position for systems biology, we will focus on developing high-resolution, high-throughput technologies for whole proteome and metabolome analysis, and enhancing strengths in microbiology, molecular biology, cell biology, and biochemistry. We will develop capabilities within EMSL around international user collaborations focused on scientific challenges in biology, physical chemistry, and biogeochemistry. Our objective is to play a key role in developing a comprehensive, quantitative, and predictive understanding of cellular and organismal functions. Under the DOE Genomics:GTL Program, we will scale our proteome and protein characterization capabilities into a new high-throughput user facility. We will manage this facility with our partner laboratories and universities as part of the set of four facilities planned for the DOE Genomics:GTL Program. To the scientific community, these newly available capabilities will enable studies of a wide variety of system-level biological problems that previously were impossible to solve.

Chemical Transformation at Complex Interfaces

Building on exceptional facilities and signatures in physical and theoretical chemistry and the geosciences, we will be recognized for our world-class research in the chemical sciences. We will emphasize research on molecular-scale behavior—the key to controlling chemistry, chemical transport, and materials properties in the condensed phase, leading to more effective separations methods for chemical
analysis; more specific, efficient, and environmentally friendly catalysts; enhanced capabilities for detecting chemical species in complex environments; and improved understanding of the migration of chemicals in natural environments.

Tools and techniques in nanoscience, chemical physics, and high-performance computing will be developed and used to understand chemical processes important to the energy and environmental sciences and the applied missions of DOE. Our investments will establish new state-of-the-art facilities in critical areas such as catalysis science and attract scientific leaders to the Laboratory. In partnership with other national laboratories and universities, we will increase our focus on fundamental research in catalysis to understand the physiochemical nature in control of catalytic activity and selectivity, and also will establish a collaborative research facility for catalysis science at PNNL.

Atmospheric Science and Global Change Research

We intend to expand our national and international leadership in atmospheric science and global change research. Our research will focus on atmospheric chemistry, continued development of the ARM Program and facilities, and on next-generation, physics-based climate models.

With our partners we will develop and implement a new program in climate physics simulation for development and testing of next-generation climate physics packages for high-resolution climate models. These new parameterizations will improve the performance of climate models and enable more accurate projections of the effects of climate change on the regional scale by explicitly describing cloud formation, precipitation, and energetics associated with cloud dynamics. We will also build upon our established expertise in integrated assessment modeling, and will develop the next generation of models for informing effective climate policy decisions.

Computational Science, Modeling, and Simulation

Critical to our success will be the development of highly impactful computational science research. We will place particular emphasis on providing a stable ultrascale computing environment as an integral component of the EMSL; advancing computer science research to ensure efficient use of ultrascale systems; and developing new methods in computational molecular science, biology, subsurface science, and climate simulation. Our long-term goals focus on developing computational methods for specific science and engineering domains or applications, along with the high-performance computing systems and infrastructure tuned for optimum performance for specific classes of computational problems.

The following modules detail specific programmatic activities and strategies we will pursue to implement our fundamental science research agenda.
2.0.1 Science Mission Funding and Staff

**PNNL estimates growth of up to 50 percent in its fundamental sciences research activities between FY 2004 and FY 2008, as well as the addition of a new user facility for Whole Proteome Analysis.**

**Key Growth Areas**

The Laboratory has a high potential for growth in SC research programs for the next five years. The most important opportunity is for growth in the DOE Genomics:GTL Program and facilities construction. We will compete for a new user facility for whole proteome analysis. Construction of this new user facility could begin in FY 2006, and it could begin operations in late FY 2008. Research within the DOE Genomics:GTL Program is also on a steep increase, and we will compete well for new multi-investigator projects within this program. Other areas of growth during this period will include opportunities in catalysis science funded by the Office of Basic Energy Sciences (BES), which could include the establishment of a facility or center of excellence, and opportunities in ultrascalar computation funded by the Office of Advanced Scientific Computing Research (ASCR).

**Office of Biological and Environmental Research**

Our increasing program presence in the biosciences is a reflection of the investments in staff, facilities, and customer relationships made over the last decade. With the completion of the Human Genome Project, biology has been expanding and the research horizons moving toward gene function, proteomics, and systems biology. We are well positioned to be a significant participant in the DOE Genomics:GTL Program. Our particular strengths are in biology of prokaryotic and microbial communities and proteomics, areas that are critical to the success of the DOE Genomics:GTL Program.

**Basic Energy Sciences, Chemical Sciences Division**

Growth potential for the Chemical Sciences programs (including Geoscience and Energy Biosciences) can be significant. The largest opportunities depend on whether or not PNNL is chosen as the site for a Catalysis Sciences User Facility/Center. In 2003, PNNL presented a proposal to the Facilities Subcommittee of the Basic Energy Sciences Advisory Committee (BESAC) outlining the research capabilities need for a user facility to enable advanced research in complex interfacial chemistry. The concepts presented have broad support among the national laboratories and universities and are focused principally on fundamental issues in catalysis. The proposal was well received by the committee with a recommendation that if such an investment were made, such a facility be competed openly among the national laboratories.
Advanced Scientific Computing Research

Significant changes in priority have occurred in ASCR with an increased emphasis in ultrascale computing, new computer architectures, and Grand Challenge research. Grand Challenge research focuses on multiple topics and, most recently, an emphasis in computational nanoscience and computational biology. While DOE has committed great effort to the development of an ultrascale program, the timing and calls for proposals and awards remain uncertain at the time of this report. We expect that this initiative will continue to focus on the high-performance computing in specific science domains; in particular, the highest priorities will be in the development of algorithms, methods, and tools that enable optimum computational performance within domain applications.

PNNL is estimating growth of approximately 50 percent in fundamental sciences research activities through FY 2008. Staff growth is projected to increase most strongly in biology, computational science, and more modestly in the physical sciences.
2.1 William R. Wiley Environmental Molecular Sciences Laboratory: Maximizing the Scientific Impact of the User Program

Within the Office of Science (SC) user facilities, EMSL has set the standard for organizing and executing collaborative research in chemistry, biochemistry, and computation. Enhancements to the EMSL user program will increase the pace and impact of scientific discovery in areas critical to DOE missions.

The science performed using EMSL facilities has helped to establish PNNL as a DOE asset for excellence in chemical, biological, and environmental sciences research. EMSL now is a very important element of our S&T agenda. To maximize the scientific productivity of the EMSL user program, we have developed three signature characteristics:

1. The integration of theory, modeling, and simulation with experiments in each of the fields where research is performed.
2. The use of multidisciplinary teams and collaborative modes of operation to solve major scientific challenges.
3. Deployment of teams of scientists/engineers to develop extraordinary tools and methodologies.

These characteristics distinguish EMSL from academic research centers and other DOE user facilities. Research using EMSL is internationally recognized for excellence in the areas of advanced computational methods, chemical physics, nanoscience and technology, oxide chemistry, high-throughput proteome analysis, structural biology, and biogeochemistry.

The long-term objectives of the EMSL user program are to:

- Operate the user facility with distinction as a best-in-class facility for fundamental research in chemistry, materials science, biology, and computation.
- Increase the impact of the user program by organizing the study of some of the most difficult and important scientific questions facing the broad research community in biology and biogeochemistry.
- Continually upgrade the capabilities/facilities to maintain a state-of-the-art research environment for the scientific community.
- Develop EMSL as the standard for collaborative research environments.

Increasing Scientific Impact Through Grand Challenges in Biogeochemistry and Biology

With program leaders at BER, we have conceived of several mechanisms to increase the impact of EMSL’s resources on the broader research community, the highest priority of which is the establishment of scientific Grand Challenge research within the EMSL user program. Beginning in 2003, we will implement scientific Grand Challenges in biogeochemistry and biology in the EMSL user program.
During its first five years of operation as a national user facility, EMSL has made a lasting scientific impact. EMSL has hosted over 2000 user projects with more than 5500 users from all continents and each of the 50 states. This use has resulted in approximately 1300 publications in archival journals.

These Grand Challenges are consistent with DOE missions, focused on critical milestones in the advancement or utilization of science. They are user-driven and take full advantage of the set of unique capabilities, resources, and technical expertise available in EMSL. The scopes of these scientific problems require multidisciplinary teaming, and are so broad that they cannot be addressed at any other existing single facility. This approach will increase the scientific impact of the EMSL as a user facility.

**Biogeochemistry Grand Challenge**

Biogeochemistry processes are fundamental to DOE mission areas of clean energy, carbon management, and waste remediation. The theme for this biogeochemistry Grand Challenge is microbe-mineral electron transfer mechanisms. The microbe-mineral interface is a complex and relatively unexplored subject. The molecular-scale mechanics and linkages across this complex region are poorly characterized and the science involved spans broad fields in biology and the physical sciences. Important scientific questions include:

- What is the structure and molecular architecture of the bacterial cell envelope-mineral surface region?
- What molecular interactions/reactions occur within this region to regulate electron flux to and from microorganisms?
- How do microorganisms sense and respond to physical and chemical shifts that occur at mineral surfaces?

The significance of this Grand Challenge topic is great and the potential impacts far-reaching. For example, it will provide BER’s Natural and Accelerated Bioremediation Research (NABIR) program the basic knowledge and concepts necessary to harness microbiological electron transfer reactions to reduce and immobilize migrating radionuclides and metals at DOE weapons sites for remedial purposes.

Maintaining EMSL’s capabilities at a world-class level and increasing the impact of its research on Grand Challenges of biogeochemistry and biology will lead to major breakthroughs in areas of S&T critical to DOE missions. Further, it will ensure that EMSL continues as the cornerstone of our S&T agenda and will help ensure that we continue building new programs and impacting new scientific areas such as systems biology.
2.2 The BER

BER is one of PNNL’s most important strategic partners in defining our science future.

Our research for BER in biology, subsurface science, and atmospheric science and global change addresses the following scientific issues:

- biotechnology solutions for clean energy, carbon sequestration, and environmental cleanup.
- low-dose radiation effects as biological systems at the molecular level
- high-throughput proteomics and analysis to enable systems biology
- response of the earth system to different levels of greenhouse gases in the atmosphere
- novel solutions to DOE’s most challenging environmental problems.

Our research contributes to each of the four divisions of BER: Life Science Research, Environmental Remediation Sciences, Climate Change Research, and Medical Sciences. Our contribution over the next five years will be focused to achieve major successes in:

- Environmental microbiology, biogeochemistry, and the development of world-class capabilities in proteomics, mass spectrometry, computation, and NMR spectroscopy and imaging. Advances in these areas will provide the foundation for new systems-level understanding of biological processes relevant to DOE missions.
- Greater accuracy in climate modeling by developing the next generation of simulation codes that explicitly describe cloud physics, and the implementation of these codes for high-performance computer systems.
- Development of the intellectual basis and technical foundations to solve currently intractable problems of contaminant fate and transport. This critical knowledge will lead to development of improved remediation strategies, and allow federal leaders to make scientifically credible risk-based decisions for environment stewardship.

The following modules detail our plans for accomplishing research for BER programs and using EMSL during the next five years. We believe that this research will contribute directly to applied programs from other offices of DOE, and for the DHS.
With support from BER, PNNL is focusing research to achieve more accurate, high-resolution climate models. By understanding the fundamental processes involved in aerosol nucleation, our researchers are fine-tuning the microphysics used in climate models, enabling more accurate predictions of not only global warming, but also climate changes and the weather.
2.2.1 Systems Biology Research in Progress

PNL will become an international leader in systems biology.

Our systems biology research focuses on the DOE Genomics:GTL Program, low-dose radiation, structural biology of bioremediation and DNA repair proteins, and innovative diagnostic and treatment technologies for biological and biomedical research. This research will increase understanding of the incredibly complex functions of whole cells and cell assemblies (e.g., microbial communities, tissues), their structures, and the networks that regulate gene expression and biological function. Our current research is focused on applying high-throughput technologies, such as proteomics and microarrays, to determine how cells and collections of cells sense and respond to their environment.

Our goal is to develop and apply advances in chemistry, physics, and computing to provide a seamless integration of experimentation, analysis, and modeling. This research will provide fundamental new molecular-level information on biological systems and provide the foundation for developing new biological technologies and processes to expedite environmental cleanup, create energy for feedstock products, and enhance human health.

Microbial Systems

Our researchers are key participants in the “Shewanella Federation,” a consortium of the DOE Genomics:GTL projects focused on a systems biology approach to the study of the biology of versatile dissimilatory metal-reducing bacterium Shewanella oneidensis. Metal reduction by microorganisms is a viable bioremediation strategy for immobilizing mobile uranium, technetium, and chromate in groundwater at DOE sites. Using a combination of 1) mutagenesis to delete key regulatory and functional genes, 2) controlled continuous culture (chemostats) methods, and 3) high-throughput array and proteome approaches, our biologists are defining the pathways and regulatory mechanisms by which S. oneidensis senses and responds to changes in electron acceptor.

With researchers from Oak Ridge National Laboratory (ORNL), we are also co-leading the DOE Genomics:GTL project focused on protein complex production and identification. We are focusing on the protein complexes from S. oneidensis.

We are also leaders in high-throughput whole proteome analysis using Fourier transform ion cyclotron resonance mass spectrometry to identify and quantify the levels of all proteins present in a cell. The technology uses “accurate mass and time” tags to identify peptides or parts of the protein as a signature of the protein’s presence and provides a level of throughput that greatly exceeds that previously possible. We can identify thousands of proteins in a single analysis, resulting in an extent of proteome coverage that is much more comprehensive than previously possible. Future advances in this technology will revolutionize biological research by enabling researchers to inventory nearly all of the proteins present in a cell at a given time and under a set of physiological conditions, and to use this information to map regulatory pathways responsible for the fundamental function of the cell.
We are also applying this technology to determine the whole proteome of various microbes including Deinococcus radiodurans and S. oneidensis. Such whole proteome analysis is critical to understanding biological systems and to revolutionizing large-scale systems biology in the 21st century. Identified by DOE as one of its four Genomics:GTL planned facilities, capabilities in Facility II (WholeProteome Analysis Facility) will focus on the high-throughput analysis of all the proteins and metabolites present in a cell under a variety of environmental conditions. Insights gained from this research are critical to developing a better understanding of biochemical networks, cell function, and gene expression for a wide variety of biological systems.

Our whole proteome analysis of D. radiodurans identified 83 percent of the predicted proteome, the most complete proteome coverage of any organism to date.

PNNL is the leader in high-throughput whole proteome analysis using Fourier transform ion cyclotron resonance mass spectrometry for identifying and quantifying the levels of all proteins present in biological systems.
2.2.1.1 Biomolecular Systems Initiative

PNNL is building expertise and infrastructure in systems biology; our research will have a profound impact on how biologists perform experiments on cellular systems, how they analyze and interpret their data, and how biological systems are described and understood.

The Biomolecular Systems Initiative (BSI) is positioning PNNL to become a leader in systems biology. While BSI is aligned with the DOE Genomics:GTL Program, the scientific capabilities under development support research projects in a variety of important areas that are beyond the scope of the program.

The four scientific thrust areas of the BSI are 1) mechanisms of microbial sensing, 2) regulation of microbial communities, 3) cellular response to oxidative stress, and 4) active cell signaling. Teams of biologists are assembled to create nationally renowned efforts in these research areas. A computational infrastructure is being built to support the research teams, including software for bioinformatics, modeling, and information management. We are also investing in new technologies for cell imaging, proteomics, and metabolite analysis. Most importantly, we are creating a cadre of interdisciplinary scientists that can productively work across scientific disciplines. These efforts, in conjunction with an aggressive collaborative outreach program, will provide outstanding new opportunities for scientific growth at PNNL.

The BSI is designed to achieve the following goals:

- Align PNNL with major new growth areas in interdisciplinary biological research and to help build strong national constituency in this area. On a national level, we will be one of the leaders in the design and creation of both an intellectual and resource infrastructure for the new field of systems biology.
- Ensure that our researchers help define the science to drive the DOE Genomics:GTL Program.
- Build the scientific expertise necessary for a strong biological sciences program in areas including molecular biology, cell biology, biochemistry, microbiology, and bioinformatics. The BSI is building specific capabilities in gene expression, gene knockout, protein expression, antibody generation, protein interactions, visualization of cell signaling, protein quantification, cell modeling, and data integration. The development of these capabilities is coordinated with the BSI’s scientific research areas to create capability “modules” that can be combined in different ways to solve a variety of problems.
- Create sophisticated, high-resolution, high-throughput technologies to help drive the development of systems biology and to exploit our strength in instrument development and automation. Pilot facilities are being constructed for high-throughput sample preparation and global proteome analyses. We are also developing the bioinformatics infrastructure to capture the enormous amount of generated data and the visualization tools to interpret it.

Examples of recent BSI accomplishments:

- A breakthrough in single-chain antibody generation, creating a “library” with more than 109 distinct types of antibodies and demonstrating a high-throughput capability to select antibodies. Now, affinity-probes may be created that are suitable for more rapidly detecting pathogens and cancer-associated pathogens.
- Successfully performing the most complete analysis of human plasma proteome, almost doubling the amount of biomarkers available for drug testing and studying health effects.
• Lead the effort to design and acquire a new facility at PNNL for global proteome and metabolite analysis of cells. This user facility is one of four proposed by DOE to support its Genomics:GTL Program and will vastly increase the current national capacity for proteomics studies in microbes. It will incorporate large-scale deployment of highly automated new technologies for whole-proteome and metabolome measurement and for imaging the distribution of proteins within living cells, and the computational tools needed to manage, analyze, and archive information on microbial proteomes under varying environmental conditions.

• Transform how scientists are able to study cells as complete biological systems, and fundamentally change the level at which biological systems can be used and manipulated for practical applications to address DOE mission needs. DHS interests include sensor applications in microfluidics and rapid detection systems of multiple pathogens. Department of Health and Human Services (DHHS) interests include improved understanding of human diseases and novel approaches to their diagnosis and treatment.

Progress

The BSI enhances S&T across the Laboratory in key areas of information technology, microscopy, and sensor development for national security, human health, and other areas. Its series of web-based resources is already improving the dissemination of information on system biology and providing access to the tools being developed at PNNL, such as antibody libraries and software (www.sysbio.org). The BSI also holds the annual Northwest Symposium on Systems Biology, and supports other workshops on systems biology and topics related to our facility efforts.

PNNL’s transgenic cells and fluorescent proteins can quantify gene expression in living cells. The ability to rapidly insert genes into normal cells and simultaneously track their distribution and activities presents many opportunities to understand the molecular basis of complex cellular networks.
2.2.2 Understanding the Effects of Energy-Related Emissions on the Atmosphere

In support of the U.S. Climate Change Program Strategic Plan and DOE’s energy and environmental missions, we conduct research to identify, understand, and anticipate the long-term health and environmental consequences of energy use and development.

Our recent climate research has led to physics-based models. This research is currently focused on the problem of climate change, and in conducting it we have made significant contributions to scientific understanding of as well as the ability to model:

- The effects of clouds on the radiative energy balance of the atmosphere.
- The effects of regional climate change on climate-sensitive natural resources and human activities. PNNL will continue this work under the climate change prediction plan and SciDAC, and may expand it into effects of aerosols or described in the next item.
- The effects of energy-related emissions on tropospheric aerosols and gas-phase chemistry on local to global scales.
- The turbulent transport of energy and mass in the atmosphere and how this transport affects atmospheric chemistry and climate.
- The roles of energy technology and energy policy in reducing carbon emissions to the atmosphere.

The ARM Program

We are a major participant in the ARM Program. The ARM Program is a DOE multilaboratory, multi-institutional effort with involvement of universities and other federal agencies. The principal goal of the program is to improve understanding of the effect of clouds on the radiative energy budget of the earth and to improve the representation of cloud processes in climate models.

The ARM Program is at a critical juncture. Through the accumulation of insights from past ARM research and through recent improvements in computational capacity, we now have the ability to implement and test new mechanisms for representing cloud processes, and their effects, in climate models. These new mechanisms enable more realistic representations of cloud processes. We intend to collaborate with university and other federal laboratory scientists who are developing new mechanisms for simulating cloud processes in climate models. We will work with these scientists in using ARM data and other climate observations to evaluate the performance of these new parameterizations in simulating observed cloud properties and effects and in improving the ability of climate models to simulate the climate system, and we will continue to do the kinds of basic research on cloud processes and aerosols that will lead to even better process parameterizations in the future. We also believe that cloud and regional-scale models can be effective tools for testing parameterization schemes and for diagnosing scale-dependent performance problems in global models. Thus, we will be working with scientists at the National Center for Atmospheric Research to use coupled
regional-scale ocean/atmosphere models to examine how the simulation of deep tropical convection and topography can affect the behavior of climate models in various difficult-to-simulate regions of the planet.

An Emphasis on Aerosols

In FY 2005, DOE will redirect its Atmospheric Science Program to an exclusive focus on the effects of atmospheric aerosols on the earth’s radiation budget. A new science plan will be developed in FY 2004; however, we expect the focus of the program will be on the microphysical, meteorological, and chemical processes that govern the optical properties of atmospheric aerosols and their effects on the optical properties of clouds. We will be directing a substantial fraction of our atmospheric science capabilities toward the support of this new program.

Through a new EMSL Collaborative Access Team (CAT), we will be partnering with leading atmospheric chemists and other atmospheric scientists in academia and industry to apply the capabilities of EMSL to the study of the complex processes of atmospheric chemistry. A major emphasis will be on processes that govern the formation and transformation of atmospheric aerosols. However, the CAT will also make these resources available to the study of other atmospheric chemistry problems of interest to DOE and other federal agencies. Detailed plans for the CAT will be developed in FY 2004, and these plans will incorporate input from non-DOE members of the research community. We expect there will be an emphasis on the development of new instruments for characterizing the chemical composition of aerosols, on improving the understanding of heterogeneous chemical reactions in the atmosphere, and on exploring the application of computational chemistry to atmospheric chemistry problems.

Measurement Tools, Techniques, and Teaming

In addition to the CAT, we will operate our Gulfstream 159 research aircraft in support of DOE research missions, and we will continue to develop state-of-the-art measurement systems, such as our Atmospheric Remote Sensing Laboratory, to support DOE’s atmospheric and climate research agenda.

We will continue to operate the Joint Global Change Research Institute in cooperation with the University of Maryland. Scientists at the institute have been leaders in the development and application of integrated assessment models for understanding the relationships among global environmental change, human welfare, and economic development. In particular, the institute will continue its research into the role of technology in reducing carbon emissions to the atmosphere. Through the institute’s Global Technology Strategy Project, we will partner with industry to identify the technologies that have the greatest promise for reducing these emissions and the strategies that can most effectively bring these technologies into widespread use.

BER has been funding PNNL since 1999 through a research consortium to conduct fundamental research on methods to enhance carbon sequestration in terrestrial ecosystems (CSiTE). These methods will be key components of a carbon management strategy to mitigate climate change. Three national laboratories (PNNL, ORNL, and Argonne National Laboratory [ANL]) and several universities participate in CSiTE. The goal of CSiTE is to discover efficient and environmentally acceptable ways to create large, long-lived carbon pools in terrestrial ecosystems.

ARM observations were used to evaluate new methods for simulating cloud radiative feedback in climate models. Net solar radiative flux at the earth’s surface, as simulated by a standard cloud parameterization scheme (top figure) and by a new technique (superparameterization) that models cloud formation and dissipation explicitly (middle), is compared to actual observations (bottom). The new method does a better job of representing the observed radiative flux.
2.2.3 The Science of Environmental Remediation

PNNL is providing the technical foundations to solve currently intractable problems of contaminant fate and transport at DOE sites, to develop improved remediation strategies, and to make scientifically credible, risk-based decisions for environmental stewardship.

Multidisciplinary, multiorganizational teams couple expertise in biology, chemistry, physics, geohydrology, applied mathematics, and computational science to address critical problems involving the molecular mechanisms of key processes, reaction and transport at the microscopic and macroscopic scales, and field-scale behavior. DOE user facilities, including EMSL and various synchrotron light sources, are used to interrogate the chemistry and structure of geologic waste materials and engineered materials, minerals, microbes, and their associations as a basis for understanding the chemical and biological processes involved.

Metal Reduction Through Microbial Processes

The principal goal of the NABIR program is to provide the scientific basis for the development of cost-effective bioremediation of radionuclides and metals in the subsurface at DOE sites. The focus of the program is on strategies leading to long-term immobilization of contaminants in place to reduce the risk to humans and the environment.

Our scientists are currently conducting research to identify the microbial and geochemical factors controlling the microbial reduction of iron and manganese, the natural substrates of dissimilatory metal-reducing bacteria, and the long-lived radionuclide contaminants technetium and uranium. Results from this research will provide important insights needed to make critical decisions regarding the cleanup of DOE sites.

For example, our researchers are examining how metal-reducing species of Shewanella can indirectly reduce soluble technetium through the enzymatic reduction of Fe(III) in mineral phases to Fe(II). Surface-associated Fe(II) in turn is able to reduce soluble technetium to an insoluble form. The role of potential competing reactions with manganese oxides and nitrate as well as the specific forms and concentrations of biogenic Fe(II) necessary to facilitate Tc(VII) reduction is being investigated in detail.

The stability of reduced technetium and uranium phases in the subsurface, specifically in regards to their susceptibility to oxidation by dissolved oxygen and subsequent remobilization, is under preliminary investigation. Issues related to re-oxidation and remobilization of metal and radionuclide contaminants is anticipated to be a major focus area in the future.
Science for Site Cleanup

DOE’s Environmental Management Science Program (EMSP) fosters the development of fundamental science and technologies for DOE site cleanup and closure. Our EMSP research portfolio is the largest of all the national laboratories, and our management approach of linking science solutions to cleanup problems has proven highly effective in our application of fundamental research for solving the complex legacy waste problems at DOE sites. Our research portfolio in support of the EMSP focuses on:

- Subsurface contaminant fate and transport.
- Remediation science.
- Nuclear waste chemistry, separations, and waste forms.
- Actinide chemistry.
- Development of novel characterization and sensor tools.

EMSP research is highly valued at the Hanford Site through our proactive efforts to engage scientific researchers directly with problems. Results from EMSP-funded efforts have provided the primary scientific bases for major corrective action decisions in Hanford’s tank farms, and will soon be used for similar purposes with river corridor plumes of uranium and Sr. EMSP research has also resolved high-visibility Hanford problems of gas generation in tank wastes and spent fuel, expedited Cs migration in the tank farms, the subsurface mineral residence and speciation of U(VI), and chemical sensors for accurate and rapid detection of technetium.

The EMSP transitioned this past year from DOE’s Office of Environmental Management (EM) to SC. A strong contingent of nationally recognized scientists in the Biological and Chemical Sciences Divisions at PNNL will provide for the continuation of its leadership role in this important program.

An EMSP workshop held at PNNL on May 6–7, 2003, brought together regulators, Hanford experts on vadose zone and groundwater contamination and tank waste, DOE Program Managers, and EMSP Principal Investigators for a scientific forum on groundwater remediation and tank waste research. The objective of this fourth-in-a-series workshop was to enhance the impact of fundamental EMSP research at Hanford by establishing strong collaborative linkages between researchers and Hanford Site problem holders.
2.3 Basic Energy Sciences

By integrating experiment with theory, modeling, and simulation, PNNL researchers have developed an internationally recognized fundamental research program focused on developing a molecular-level understanding of complex chemical and material systems and phenomena important to the nation’s energy, environmental, and security needs.

With scientific expertise in molecular and nanoscale science, engineering, and technology and high-performance computing, our scientists are enabling an atomic and molecular-level understanding of complex multiphase chemical, material, and nanoscale systems. As part of multidisciplinary, multi-institutional teams, we will provide the conceptual framework and the experimental and computational tools required to understand chemical transformation at interfaces and photonic and molecularly assembled nanostructural materials.

DOE user facilities, especially the EMSL and the various synchrotron light sources at other national laboratories, are critical to this program. We anticipate increased application of neutron scattering. Application of our unique high-throughput proteomics and metabolomics capabilities to problems in energy biosciences is also anticipated.

Chemical Sciences

The Chemical Sciences research program focuses on condensed phase and interfacial chemical physics (especially in aqueous systems), advanced methods of separations and analysis (particularly mass spectrometry, ionic processes, and the chemistry and physics of nanoparticles), and catalysis and chemical transformation (especially at nanostructured interfaces and in confined local environments).

Based on our strengths in these and other areas, we anticipate making significant contributions to DOE’s Grand Challenge of developing the increased understanding required to design catalyst structures to control catalytic activity and selectivity. Key to successful realization of this Grand Challenge goal will be the development and application of an integrated suite of advanced experimental and computational resources to model, design, synthesize, and characterize kinetically and dynamically in situ catalysts from the nanoscale to the macroscale. Such advanced resources are not available to the community of catalysis scientists today, nor are they part of any planned user facility (including the Nanoscale Science Research Centers currently under development). The Complex Interfacial Catalysis Facility proposed by PNNL in 2003 would fill this need.

(a) This Grand Challenge is articulated in the 2003 BESAC report entitled Opportunities for Catalysis in the 21st Century.
**Geosciences**

The Geosciences research program focuses on unraveling the fundamental biogeochemical interactions between minerals, solutions, and microorganisms that occur in geologic environments and control the transport and fate of contaminants in the environment. The program emphasizes developing a molecular-level understanding of these interactions through the use of advanced surface spectroscopies and molecular and thermodynamic modeling simulations. Current areas of study include:

- developing molecular models for describing iron oxide surfaces and adsorption reactions
- unraveling the molecular-to-micron-scale reactions at carbonate surfaces
- developing molecular models for lipopolysaccharides present on the outer surface of environmentally important bacteria
- understanding the role of microorganisms in iron reduction and their attachment to mineral surfaces.

Future research plans are in the areas of nanogeo science, neutron research, and in investigating the influence of transport on reactivity at the nano to micron scale.

**Materials Sciences**

Core projects within the Materials Sciences program suite focus on developing innovative synthesis and processing methods, modeling and affirming structure property relationships particularly in materials containing intentionally introduced defects, investigating materials-environment interactions at the atomistic level, and using molecular probes such as NMR in consort with beam techniques available at the DOE user facilities to characterize structural nuances at different length scales. Building on previous program successes, PNNL’s evolving materials science research activities focus on molecular assembly routes to nano-architected materials, the design of photonic materials that exhibit a predicted and reversible response to light, and a new class of spin transport oxide films to enable next-generation computers.

PNNL’s dynamic research team integrates theory with experiment, pursues leading-edge research centered on the formation of defects in materials, and the role of defects in molecular adsorption on, chemical reactivity at, and charge transport through oxide surfaces. Results of this research will influence science directions that significantly impact DOE mission areas ranging from waste sequestration; to energy storage, generation, and transformation; to infrastructure reliability.

Support from BES allows researchers at PNNL to make significant contributions to nanoscale and molecular research in the areas of chemical sciences, geosciences, and materials sciences. Here, PNNL researchers use the state-of-the-art molecular beam epitaxy system housed in the EMSL to create a continuous thin film of metal layer on metal oxide.
2.3.1 Nanoscience and Technology Initiative

The Nanoscience and Technology Initiative (NSTI) creates the capability to manipulate structures at an atomic scale, enabling fundamental changes to the properties of materials and making possible new materials, chemistry, and functions.

Nanoscience is the investigation of phenomena that occur on the nanoscale (0.1 to 100 nanometer); nanotechnology is the application of these phenomena. Our researchers seek to create functional materials, devices, and systems by controlling matter on the nanometer scale to exploit novel phenomena and properties (physical, chemical, biological) at this scale. For instance, the manipulation of electronic structure to produce chemically tailored surfaces promises substantial advances in several application areas critical to DOE missions.

The first and broadest of these areas is catalysis, where chemically active nanostructures facilitate environmental remediation, enable the clean production of hydrogen (and may play a key role in new hydrogen storage media), and control the direct reaction of chemical feedstocks with oxygen to produce electricity in high-efficiency fuel cells. The second key area is high-specificity detection of chemical, biological, and nuclear agents. Here, the tunable chemistry of nanoparticles, particularly nanobiological structures such as enzymes, promise simultaneous high sensitivity and a high-rejection ratio of chemically similar but benign species. The high-surface-area-to-volume ratio intrinsic to nanostructures enables further development in active preconcentrators for analyte treatment prior to detection.

The NSTI is crosscutting, and interdisciplinary priorities for the initiative are as follows:

- Understand chemical interactions at the nanoscale, enabling the tailoring of chemically functional surfaces using “bottom-up” assembly techniques.
- Develop a core scientific strength in nano-catalysis including controlled synthesis, characterization, and modeling techniques to understand single-site reactivity.
- Develop the field of nanobiology, focusing on biocatalysis and the use of enzyme-based nanoparticles for detection and remediation of contaminants.
- Increase the visibility of nanoscale research at PNNL both regionally and nationally via leadership of symposia and workshops, hosting visiting scientists, and promoting the use of EMSL for collaborative research in nanoscience.
- Operate the Joint Institute for Nanoscience with the University of Washington and form a broader umbrella organization for nanoscience in the Pacific Northwest.

Examples of recent Nanoscience and Technology Initiative accomplishments:

- Developed a new class of thin film epitaxial magnetic semiconductors based on doped conductive oxides which retain magnetization significantly above room temperature, enabling future spintronic devices.
- Demonstrated composite nanobiological materials with potential applications in catalysis and detection. Single enzyme nanoparticles are modified natural enzymes armored with a synthetic silicate shell that extends by orders of magnitude the lifetime of the enzyme without destroying its activity.
Nanoscience is an interdisciplinary research field at the interfaces of physics, chemistry, and biology. The NSTI is similarly interdisciplinary and crosscutting and, as such, targets growth in several PNNL programs, specifically:

- SC: Early work funded by NSTI has transitioned to programmatic support from both divisions of BES and EMSP. Current and future projects will develop capability to support a significant new catalysis facility.

- DOE Office of Energy Efficiency and Renewable Energy (EERE): Nanocatalysis projects with a particular emphasis on improved fuel cell efficiency and hydrogen production and storage are part of NSTI.

- DHS: In collaboration with the Homeland Security Initiative, NSTI is building the capability to use the tunable chemistry and high surface area of nanostructures to selectively adsorb and detect analytes at low concentration.

This figure illustrates the concept of hierarchical assembly for tailored functionality. Nanoscience revolutionizes the way we think about making materials. Until recently, we were limited to starting with naturally occurring (bulk) materials and using tools to shape them into useful products. This is called “top-down” fabrication. Using nanoscale engineering, we create molecules with desired functionality and invoke molecular-level forces to cause them to assemble themselves into clusters or layers (“bottom-up” fabrication), yielding new tailored materials that could not be produced by top-down techniques.
2.4 Computational Science and Applied Mathematics: Scaling Computation to Meet Science Challenges

PNRL researchers will achieve better accuracy, resolution, and simulation fidelity in modeling physical systems by developing new mathematical and computational methods that integrate physical phenomena across wide scales of distance and time.

Computational science applications and systems must scale with problem size, accuracy requirements, computer capability, number of collaborators, data volume, and number of datasets. Efficiently and effectively employing both the current and next-generation massively parallel computers, massive databases, and high-speed communications requires advances in programming models, system software, collaboratory and grid middleware, computational mesh tools, data transport, numerical algorithms, statistical approaches, and data visualization techniques. Therefore, our successful computational science efforts require a robust set of crosscutting fundamental research capabilities in computer science, applied mathematics, and statistics.

Advanced Scientific and Computational Research

With an established nucleus of programs and senior investigators, we will strengthen our capabilities and programs in the areas described above by building staff and program depth with the ASCR. During the next several years, our major thrusts are keyed to research aligned with the research program thrusts of ASCR.

- We will continue to carry out and diversify research programs that are creating efficient and productive programming environments and systems software for scientific applications on the very largest computer systems, including first-of-a-kind computational infrastructure. These tools are integral to research in EMSL’s Molecular Science Computing Facility and to research programs in nanoscience, bioinformatics, climate physics, and subsurface transport, to name a few.

- We will continue to develop scalable, adaptive mesh refinement techniques to enable computational models of new classes of systems. These capabilities are core components of computational applications in cellular biology, organ modeling, and nanoscience, with future application to materials science and computational engineering. They are also integral to comprehensive modeling tool suites being developed with our collaborators for SC applications.

- We will develop new basic research projects in mathematical and statistical methods to deal with the scale and complexity of large science problems, with emphases in bioinformatics analysis, informatics for homeland security, environmental risk assessment, and model uncertainty in contaminant transport.
- To improve the ability of researchers to interact with very large datasets, we will develop new research programs directed at creating interactive visual analysis techniques that accelerate discovery with new approaches to scientist-information interaction. Our initial science application targets include the systems biology of microbes, and the analysis of regional and global climate models.

- To enable scientists to productively use widely distributed computing resources and databases, and to collaborate with experts regardless of their location, we will continue our research thrusts and pilot projects in architectures and middleware for collaborative problem-solving environments. These tools will enable new approaches to distributed science efforts in a wide range of mission areas, with current emphases in protein structure, systems biology, and chemistry.

- PNNL will be a full partner in the DOE Science Grid. We will provide and support grid services on our major computer facilities for science research (e.g., the 11.8-teraflop computer in the EMSL). PNNL will continue to participate in the development of grid systems, tools, and policies to further the reach and accessibility of computational science applications and data.

Although this work is primarily directed toward ASCR capabilities, it also leverages investments in new computer science, applied mathematics, and statistics capabilities being developed in our Computational Sciences and Engineering Initiative, as described in Module 2.4.1.

Efficient, scalable mesh-based computational techniques are essential for modeling a wide range of biological systems from signal propagation in microbes (above), to aerosol particle movement in lungs, to salmon interactions with dam structures. PNNL is developing adaptive mesh refinement capabilities as part of a multi-institution collaboration in Terascale Simulation Tools and Technology, an ASCR applied mathematics Integrated Software Infrastructure Center in the Scientific Discovery Through Advanced Computing Program.
2.4.1 Computational Sciences and Engineering Initiative

The Computational Sciences and Engineering Initiative (CS&EI) will develop advanced modeling and simulation capabilities that will be broadly used by PNNL’s R&D programs.

Computational science is an integral capability required throughout the Laboratory and is key to our future success. Through CS&EI, we will develop special capabilities for computational science in specific core areas to achieving the vision for the Laboratory, including chemistry, biology, climate, remediation, and national security. Our long-term goals focus on developing a series of major modeling and simulation suites for specific science and engineering domains, along with high-performance computing systems and infrastructure that are optimized for these suites, and the underlying support for these capabilities and their users.

An overarching scientific theme of CS&EI is developing computational capabilities across PNNL mission areas that deal with complex behavior on different temporal and spatial scales, and that enable us to carry out the demanding and sophisticated simulation, modeling, and analysis necessary to distinguish our research programs in chemistry, biology, atmospheric sciences, national security, materials engineering, and subsurface science.

Computational science draws upon and blends the advanced skills of many domains. Success requires strong capabilities in core areas of computer science, applied mathematics, and statistics. In addition, a core infrastructure of networks and computers is required to meet the computational demands of the scientific domains.

This initiative is characterized by:

- Creating new modeling, simulation, and analysis techniques that expand the boundaries of the study of complex systems essential to our missions in chemistry, bioinformatics, subsurface transport, nanoscience, materials engineering, and information analytics.
- Developing innovative computer science, mathematics, and statistics approaches for highly effective and efficient use of tera- to peta-scale computing, sophisticated problem-solving environments, and massive data analyses that minimize time to solution and accelerate scientific discovery.
- Providing advocacy and leadership for forefront computational facilities, state-of-the-art networks, and other technical computing infrastructure needed to serve PNNL and the external user communities in support of our science and engineering programs.
- Increasing the visibility of our computational science and engineering activities and capabilities throughout the science community through peer-reviewed publications, seminars, visiting scientists, technology exhibitions, and scientific symposia/workshops.

Example of recent CS&EI accomplishments:

- Demonstrated self-consistent-charge density functional tight-binding models to include atomic forces, and coupled them to drivers for energy minimization, transition-state determination, force-constant calculation, and molecular dynamics simulations. This permits quantum modeling and simulation of systems that are at the heart of biochemical reactivity and nanoscale science.
- Completed the development and implementation of a damage model for short-fiber composites using a multiscale mechanistic approach.
- Developed a novel visual data mining method to provide exploration and navigation capabilities to our ongoing whole-genome alignments work.
Because the focus of this initiative spans missions in each of the Laboratory’s directorates, a wide range of our programs are targeted for substantial growth, with major emphasis on the following research programs:

- Key roles in the new ASCR science computing initiative planned for FY 2005; defining new programs in subsurface science simulation, climate physics, computational biology and bioinformatics in BER and ASCR; and extending the impact of computational chemistry and computational nanoscience in BES.
- EERE programs in lightweight materials and hydrogen fuel systems.
- DOE and DHS programs in homeland security, with an emphasis on dynamic information analysis in collaboration with Homeland Security Initiative (see Module 4.5.1).

High-resolution clastic dike simulation yields new insights on vadose zone transport. At the Hanford Site, the presence of vertical clastic intrusions has raised concerns over potential expedited contaminant transport pathways through the vadose zone. In conjunction with millimeter-scale geophysical measurements, high-resolution simulations of flow, and reactive transport using parallel processing subsurface simulators have identified distinct and complementary pathways under natural and leaking conditions. Contaminants present in the leaking events may be considerably less mobile when natural conditions return.

Example of recent CS&EI accomplishments (contd):

- Completed a one-dimensional test problem involving the migration of carbon tetrachloride through Hanford soils using the parallel implementation of the Water-Air-Oil operational mode of the Subsurface Transport Over Multiple Phases (STOMP) simulator on the Molecular Science Computing Facility supercomputer. A three-dimensional test problem developed under the Hanford Science and Technology project was used for the final verification of the parallel implementation of the Water-Air-Oil operational mode of the STOMP simulator. The successful execution of these three-dimensional simulations on multiprocessor computers completed the development and demonstration requirements for the parallel implementation of the Water-Air-Oil operational mode.
2.5 Research for the Department of Health and Human Services

Growing research supported by the National Institutes of Health (NIH) is aligned with the Laboratory vision to build an internationally recognized program in systems biology.

Our systems biology approach that integrates experimental biology with the physical and computational sciences is attracting support from NIH programs and is an example of beneficial leveraging of the strengths among DOE and other federal agencies. Our ability to translate fundamental research to application forms the base for establishing relationships with the Centers for Disease Control and other DHHS programs beyond the NIH. DHHS is becoming a critical partner in carrying out successful cross-disciplinary and multi-institutional research in systems biology centered on our capabilities in structural biology, molecular and cellular imaging, high-throughput global proteomics, and bioinformatics and computational biology.

The continued development of NIH programs relies on our state-of-the-art capabilities. Growth in the scientific impact of our NIH research depends on the unique capabilities of the proposed facility for high-throughput proteomics and metabolomics, and also builds on existing research strengths in cell signaling, structural genomics, molecular toxicology, and microbiology. The awarding in 2003 of a large, multiyear National Center for Research Resources project in mass spectrometry to PNNL to support research in proteomics across the NIH is evidence that the leading-edge technology being developed in EMSL is recognized by the biomedical community.

Under the BSI, PNNL has leveraged the investments in developing capabilities supporting DOE programs to build an NIH portfolio of investigator-initiated projects focused on fundamental cell biology. The Laboratory now plans to use this base to develop larger, multi-institutional program projects with NIH support, such as the ongoing Superfund Basic Research Center project funded by the National Institute of Environmental Health Sciences (NIEHS) in collaboration with the Oregon Health and Science University and Oregon State University.

Human Health Research

The Laboratory also conducts applied research and technology development in support of the DHHS human health mission. Monitoring workers for chemical exposures during environmental cleanup is an important DOE issue and a critical scientific challenge. We are developing real-time, noninvasive biomonitors that can be used to measure chemical exposures to workers by integrating systems biology with our strengths in personnel dosimetry, chemical toxicology, microtechnology, and sensors. The National Institute for Occupational Safety and Health is funding research projects that further develop this technology and study exposure to dose to health effects in selected populations.
With support from NIEHS, our scientists identified or confirmed 490 proteins in human blood serum, nearly doubling the number of known serum proteins. Blood serum holds clues to all the major processes in our bodies; by knowing what proteins exist in that serum, it may be possible to predict disease susceptibility, monitor disease progression, or diagnose disease.

“After a long period of slow progress, research on the plasma proteome has begun a period of explosive growth attributable to new multidimensional fractionation methods,” said N. Leigh Anderson, founder and chief executive officer of The Plasma Proteome Institute. “PNNL’s work is an important early demonstration of the power of these methods, and suggests that hundreds, if not thousands, of new candidate markers will be found.”

Relative abundance of the proteins that make up 99 percent of the protein mass in blood plasma. The final 1 percent represents thousands of proteins (Image courtesy of Plasma Proteome Institute).


2.6 New Whole Proteome Analysis Facility for Systems Biology

A critical aspect of the DOE Genomics:GTL Program is the establishment of four major scientific facilities. PNNL is developing a proposal to build and operate one of these, the Whole Proteome Analysis Facility.

The DOE Genomics:GTL Program is an ambitious program to achieve a fundamental, comprehensive, and systematic understanding of microbial life. As noted in DOE’s Genomes to Life: Realizing the Potential of the Genome Revolution document, “GTL is designed to help launch biology onto a new trajectory to comprehensively understand cellular processes in a realistic context. This new level of exploration, known as systems biology, will empower scientists to pursue completely new approaches to discovery, transforming biology to a more quantitative and predictive science.” Major research projects were initiated in FY 2002 and proposals in response to a second call were submitted in April 2003. Along with this substantial programmatic research commitment, DOE determined the need for four major new scientific facilities.

These facilities will use advanced high-throughput technologies, will be highly automated, and will include tools necessary for building an integrated environment of software for data management, analysis, and simulation. DOE intends to provide open access to these facilities as well as the data they generate—“a plan to democratize access to systems biology resources.” The four planned facilities are: I. Production and Characterization of Proteins Facility; II. Whole Proteome Analysis Facility; III. Characterization and Imaging of Molecular Machines Facility, and IV. Analysis and Modeling of Cellular Systems Facility.

We are in a very competitive position for facility II because of our key expertise in microbiology, proteomics, and advanced analytical technologies and tools, such as high-field mass spectrometry and NMR imaging, advanced data visualization environments, and high-performance computing.

Additional Biology Prototype Facilities Needed

The DOE Genomics:GTL facility development effort is an integral element of our BSI. As discussed in Module 2.2.1.1, BSI is investing in critical scientific programs and capabilities in proteomics and is providing support for the development, delivery, and operations of this facility. An important part of this support is the creation of two biology prototype facilities. One is the Proteomics Sample Processing Facility in PNNL’s LSL-2 Building, and the other is the Microbial Cell Dynamics Facility currently in the 331 Building. Plans are under development to expand these prototypes to further support the DOE Genomics:GTL Program facility development efforts.
Preparing to Win

We are establishing the significant partnerships, constituents, and advocacy required to be successful throughout the DOE Genomics:GTL Program facility-development process. Building and operating the Whole Proteome Analysis Facility is a critical long-term goal for the Laboratory. Near-term efforts to achieve this goal consist of the following:

- holding workshops/technical exchanges on various scientific, technical, and operations aspects of the facility to refine the facility concept and establish appropriate third-party relationships
- establishing a pilot high-throughput production facility for protein and metabolite analysis inclusive of critical research and development efforts
- expanding the two PNNL biology prototype facilities as a part of establishing the pilot production facility
- continuing with the appropriate BSI programs and investments
- hiring/identifying key persons to lead various aspects of the facility development
- continuing work with DOE and national laboratories, universities, private organizations, and others, to be positioned to successfully compete for the Whole Proteome Analysis Facility.

To support the DOE Genomics:GTL Program, PNNL is proposing to build and operate Facility II — the Whole Proteome Analysis Facility. The facility concept is a production-oriented laboratory that merges with nonlaboratory space to facilitate collaboration, communication, and access with the scientific community.
3—Energy
3.0 PNNL’s Role in DOE’s Energy Research Mission

PNNL will expand scientific knowledge and create breakthrough technologies for the energy system of the future, enabling secure, clean, and affordable energy in a carbon-constrained world.

Our R&D in support of DOE’s energy mission is aligned with two parallel paths—one that focuses on using existing resources in the most efficient and environmentally acceptable manner possible, and one that focuses on bridging the gap between today’s energy systems and tomorrow’s hydrogen economy. Our unique combination of multidisciplinary capabilities and a vision of the energy system of the future positions us for leadership in developing a comprehensive, intelligent national grid that includes energy generation, transmission, distribution, and end use in industry, in the home, and transportation. By combining information, simulation, and visualization technologies with new energy technologies, we will increase the nation’s energy security and reliability, dramatically reducing the need for expensive new energy infrastructure.

Developing Technologies for Clean and Efficient Power Generation

We develop technologies for meeting growing energy demands in ways that are economically viable, minimize the release of greenhouse gases, and reduce our dependence on imported oil. While we are exploring a transition to a hydrogen economy, our near-term efforts will focus on maximizing energy efficiency, increasing the use of renewable energy, and using nonrenewable resources in environmentally acceptable, economic ways. For example, our fuel cell technologies, our scientific understanding of thermoelectric materials, and our carbon sequestration analyses and pilot projects are relevant to DOE’s FutureGen program, aimed at constructing the next-generation fossil fuel energy plant (Module 3.3). Through our participation and leadership in the Solid State Energy Conversion Alliance (SECA, Module 3.3.1), we will strive to reduce the cost of solid oxide fuel cells by 50 percent. Nuclear power currently provides about 20 percent of the nation’s electrical generating capacity; our material scientists are recognized world leaders in evaluating the ability of existing nuclear power plants to extend their operating licenses to produce electricity without generating greenhouse gases.

Expanding Bio-Based Products

In support of the nation’s need to reduce its dependence on imported oil, our researchers are exploring technologies to make bio-based products and fuels more prevalent and economically viable (Module 3.1.3). Building upon our expertise in catalysis, we conduct research to transform agricultural byproducts into high-value chemicals and products, which supports the Office of Energy Efficiency and Renewable Energy’s (EERE) goal to create a $1 billion annual bioproducts business in the United States.
Developing Hydrogen Systems

To encourage a successful transition to a hydrogen economy, we bring together policy and analysis expertise as well as scientific capabilities that are directly applicable to the challenges associated with hydrogen production, storage, distribution, and safety (Module 3.1.1). In 2003, we were assigned leadership of DOE’s hydrogen safety program. During the next several years, we will conduct integrated analysis and evaluation of hydrogen systems as part of the President’s Hydrogen Initiative.

Leading the Vision of the Grid of the Future

Our vision of the grid of the future, known as GridWise™, will harness the power of information technology and new energy technologies to transform the energy system into one that is intelligent, robust, reliable, and secure. This vision addresses national needs by modernizing the energy system into the information age, making it possible to 1) reduce the need for expensive infrastructure, 2) incorporate and value the contributions of distributed energy solutions, 3) increase the security of critical infrastructure, and 4) visualize the system in ways that makes it understandable, manageable, and transparent to system operators and regulators. We are particularly well-suited to integrate this vision because of our scientific capabilities and experience with practical applications related to many aspects of the energy system. These capabilities include modeling and computation, grid reliability, materials science, development of fuel cells and other innovative energy technologies, and economics and policy analysis. This comprehensive, intelligent national grid has the potential to save the nation nearly $80 billion of the roughly $450 billion of projected investment needed in energy infrastructure to accommodate growth over the next 20 years.

Advancing Transportation Technologies

Based upon our materials, catalysis, and surface interaction science, we are developing advanced technologies for transportation, such as lightweight materials, solid oxide fuel cells, and emission aftertreatment technologies for passenger vehicles and trucks (Module 3.1.2). These technologies help increase fuel efficiency and reduce emissions in the transportation sector, which is responsible for a third of the nation’s carbon dioxide emissions and today relies almost entirely upon fossil fuels.

Primary Energy Customers

Our energy-related R&D supports the needs of several offices within DOE, including EERE (Modules 3.1 – 3.1.4); the Office of Fossil Energy (FE, Modules 3.3 and 3.3.1); and the Office of Nuclear Energy, Science, and Technology (NE, Module 3.5); as well as the newly formed Office of Electric Transmission and Distribution (OETD, Module 3.2) and DOE’s Climate Change Technology Initiative (CCTI, Module 3.4).

The programs and initiatives described throughout Chapter 3 of this Institutional Plan discuss how PNNL supports DOE in providing secure, clean, and affordable energy, and are closely aligned with the Laboratory Agenda items, shown here.
3.0.1 Energy Mission Funding and Staff

PNNL estimates 35 percent growth in its energy mission activities between FY 2002 and FY 2008.

Key Growth Areas

The majority of our energy business and new opportunities will come from EERE. While a smaller component of our overall energy business, support for FE will nearly double by FY 2008. Funding from NE will likely see the most modest growth.

Energy Efficiency and Renewable Energy

The largest areas of growth for PNNL within EERE relate to biomass research, hydrogen, and fuel cells. This business may expand by much as to $15 million during the next five years. These areas of expected growth are aligned with national initiatives, as well as Laboratory initiatives supported by internal investments. Projects that traditionally fall within the Distributed Energy and Electricity Reliability program will also see significant growth; however, because of reorganization within DOE, most of this research and development will eventually be moved to OETD (Module 3.2). This new office will include research related to the grid of the future and the reliability of the electricity infrastructure.

Within EERE, we expect to see decreased funding over time within the Federal Energy Management Program and Weatherization. Our relative portion of these overall budgets are expected to remain about the same during the FY 2004–2008 planning period, but trends indicate a shift in the federal government’s priorities and dramatic decreases in DOE’s overall budgets in these areas. For example, the Federal Energy Management Program budgets at the national level are being reduced by 15 percent in FY 2004. Even so, we will work to preserve our core business in these areas because these resources and our related capabilities are critical to our ability to build business in other areas of growth.

Fossil Energy

Three key areas of funding for our energy research from FE are expected to see growth during the FY 2004–2008 planning period: the SECA, the High Temperature Electrochemistry Center, and carbon management and sequestration. These three areas all support FE’s FutureGen Initiative (Module 3.3), which aims to build the energy-efficient, emission-free fossil energy plants of the future.

Our expanding relationships with collaborators such as NASA and Boeing in the area of solid oxide fuel cells may bring new revenues to the Laboratory and shore up impactful funding sources. However, achieving the targets for growth in funding directly from FE projected on the chart shown here will require new business areas, such as carbon management and carbon sequestration demonstration projects or emission research. During the next five-year planning period, a portion of the work traditionally designated as part of FE will be aligned with the newly created CCTI within DOE (Module 3.4).
Nuclear Energy, Science, and Technology

While we project modest growth in funding from NE, achieving these targets will require that we move into program areas such as space power, next-generation reactors, or reprocessing—new programs that are not currently receiving significant funding. We plan to build on our experience and strengths related to understanding the effects of radiation on materials.

Work for Others

Our energy research for other government agencies and industries (Module 3.6) includes work for:

- Bonneville Power Administration (BPA)
- U.S. Nuclear Regulatory Commission (NRC), where we expect modest growth
- Energy companies, where we expect to see increases over the planning period
- European Bank for Reconstruction and Development.

Resources aligned with the private energy industry focus primarily on work related to the automotive industry, industrial partnerships related to carbon sequestration, opportunities for new hydrogen demonstration projects, and collaborations with utilities and other private companies in pursuit of an energy system transformation or part of the GridWise activities (Module 3.2.1).

One reason for a slight decrease in this sector is that over time, we expect the work related to the former Soviet Union and nuclear reactor safety to decline as the first phase of planning and consulting related to projects under the European Bank for Reconstruction and Development (including the new safe confinement of the Chornobyl reactor) is completed. In part, these decreases are expected because more European support is available to implement the plans and complete long-term projects.

All PNNL energy mission areas show steady growth through 2007.
3.1 Maximizing Energy Efficiency and the Use of Renewable Energy

PNNL will strengthen America’s energy security, environmental quality, and economic vitality by applying its capabilities to increase the use of renewable energy and maximize energy efficiency.

With a long history of funding from EERE and strong linkages to private industry, we are enhancing energy efficiency and productivity, bringing clean, reliable, and affordable energy technologies to the marketplace, and reducing America’s dependence on imported oil. Our scientific and technological contributions in this area are aligned with DOE’s vision for the energy future that includes:

- increasing efficiency in cars and trucks and powering them with clean domestic fuels
- reducing energy costs and increasing efficiency for homes and industry
- revitalizing the electricity infrastructure, making it more robust and reliable
- increasing the use of renewable resources and the quantity of power generated by homes, businesses, and communities and sold back to local generators
- creating industrial energy parks that use and produce energy
- improving the economy for rural America through biomass feedstocks for biorefineries that produce power, fuels, chemicals, and other valuable products
- developing leadership in conserving energy and using renewable energy resources within the federal government.

Strategic Integration

Our expertise in surface characterization and catalysis, systems integration and analysis, modeling and simulation, and diagnostics and prognostics provides a strong foundation that directly supports DOE mission needs related to renewable energy and energy efficiency. We also are building our scientific capabilities in electrical engineering and economics to help bolster the transformation of the electrical infrastructure. We are pursuing an opportunity to bring together several disparate pieces and legacy programs, including several funded by EERE and some now managed by OETD (see Module 3.2), under a single strategy for the energy system of the future. This strategy integrates energy generation, demand management and distribution, and environmental concerns to meet the electricity demands of today, and the use of hydrogen for distributed generation and transportation in the future.

Partnerships, Collaborations, and Leveraging Resources

Regional partnerships play an important role in our support to EERE’s mission. For example, we were a founding member of the Northwest Energy Technology Collaborative, formed in 2002 to accelerate the growth of the energy technology industry in the Pacific Northwest. This partnership includes the Washington Technology Center, Avista Corporation, BPA, Spokane Intercollegiate Research and Technology Institute, the Washington State Office of Trade and Economic Development, and the Inland Northwest Technology Education Center.
We will continue to invest internal resources to improve our ability to respond to DOE's needs and will continue to rely on our strong linkages with industry to leverage funding from EERE, as well as funding from FE, the Office of Science (SC), and the Office of Basic Energy Sciences (BES) to further advance energy technologies in solid oxide fuel cell research, vehicle technologies, and microtechnologies. For example, we are leveraging FE’s SECA (Module 3.3.1) and our leadership in this alliance to pursue the development of solid oxide fuel cells for transportation and auxiliary power.

We also will use SC facilities at the Laboratory for EERE missions such as furthering our understanding of emission chemistry in the atmosphere and its impacts on human health.

PNNL is committed to improving the energy efficiency of U.S. industry by delivering high-quality R&D on advanced process systems, advanced industrial materials, and chemical and enabling technologies. Our program aims to build collaborative teams with industrial partners throughout the United States to leverage their expertise and drive commercialization of our technology. For example, our largest project in FY 2004 teams with five organizations, and focuses on developing low-cost thermoelectric systems with 20 to 40 percent efficiency for recovering waste heat in process industries and vehicle exhaust systems. This research will include thin film design, multilayer chemistry and tailored interfaces, and thermal and electrical modeling.

Wind and Hydropower Technologies

Our scientists also conduct R&D aimed at building more environmentally friendly technologies to maintain the nation’s existing hydropower capacity in support of the Office of Wind and Hydropower Technologies. For example, we help define biological specifications for safe operation of hydropower turbines and test turbine design and modifications. In the next five years, we will coordinate our research portfolio in this area to include the BPA, the Western Area Power Administration, private utilities, and the Army Corps of Engineers.

Planning and Analysis

PNNL also provides analysis and process development to EERE. Our activities in this area include evaluating energy impacts of past programs, assessing potential impacts of new programs, and providing integral support to the multiyear planning process.

PNNL applies its expertise in surface chemistry and catalysis to develop technologies that reduce harmful emissions from diesel engine exhaust, converting oxides of nitrogen and particulate matter into components of clean air. These same surface chemistry capabilities will be valuable in addressing technical challenges related to bio-based products and fuels, vehicle technologies, carbon capture and sequestration, and advanced energy systems.
3.1.1 Hydrogen S&T

PNL will lead the hydrogen safety program and make advances in S&T for a hydrogen economy of the future, helping the United States lead the world in developing clean, hydrogen-powered automobiles, and in the development of hydrogen production, storage, and delivery technologies.

The President announced two initiatives in 2003 related to hydrogen: the Hydrogen Fuel Initiative and FutureGen (Module 3.3). Paving the way for hydrogen’s rapid growth as an energy carrier over the next several decades will require achieving the goals of hydrogen technology and favorable regulations and policies.

Our internal investments and programmatic efforts in hydrogen R&D have positioned us to become a key provider of cutting-edge S&T relevant to the national hydrogen program, including:

- hydrogen storage materials
- hydrogen production technologies
- science and engineering in support of hydrogen safety
- reforming technologies and auxiliary power units and sensors.

We are also engaged in establishing regional collaborations that deal with deployment and testing of the hydrogen system of the future.

Production

We are developing technological solutions for the production of hydrogen from diverse renewable sources. The following attractive and technically viable approaches build on current laboratory capabilities.

- **High-temperature steam electrolysis**, which has the potential to reduce substantially the electrical requirements to convert water into hydrogen and oxygen. We will build on our capabilities in planar solid oxide fuel cells and the High-Temperature Electrochemistry Center in pursuit of this option (Modules 3.3.1 and 3.3).

- **Gasification of biomass feedstocks**, which uses high-activity catalysts in water solvents at moderate temperatures and pressures. We will build on our expertise in catalysis, reactors, and feedstock conversions to extend the scope of bio-based products research (Module 3.1.3.1) from high-value chemicals to hydrogen production.

- **Photocatalyzed water splitting using single-cell algae**, in which hydrogen and oxygen production are physically separated, avoiding one of the most challenging issues in bio-photocatalysis. We will build on our expertise in genetic modification to increase productivity of the algae.
Storage

The hydrogen storage challenge must be addressed for a hydrogen economy to be realized. Using today's technology, vehicles could carry only enough hydrogen to travel about 150 miles— the goal is to be able to travel 300 miles. To accomplish this goal, new materials are needed that provide volumetric and storage capacity, or further understanding of existing materials to increase their storage capacity. We are teaming with Los Alamos National Laboratory on a proposal to establish a center-of-excellence for research on chemical hydride storage materials. Such a center will take advantage of our experimental, characterization, and computational chemistry capabilities (Module 2.4.1) and the capabilities being developed as part of the Nanoscience and Technology Initiative (Module 2.3.1). We also have begun capability-development projects to further develop our understanding of the fundamental mechanisms of hydrogen storage in metal hydrides. SC and EERE are teaming on the development of advances that require basic understanding of materials.

Safety

Hydrogen is a new fuel for widespread use; therefore, there is a need to establish codes and standards and to increase awareness and the public perception related to its safety. We have been designated by DOE's Fuel Cells, Hydrogen, and Infrastructure Program as the national lead for the hydrogen safety program. An integrated approach to safety will establish crosscutting activities that identify all aspects of risk and effectively and economically address them. As part of leading the integrated safety program, we will test hydrogen systems, develop sensors to detect hydrogen leaks, and establish best practices for hydrogen safety. We also will continue exploring the possibility of using the Hazardous Materials Management and Emergency Response (HAMMER) training facility in Richland, Washington, as the main facility in the nation for hydrogen safety training of fire marshals and code officials. In addition to supporting the DOE's hydrogen programs, integrated hydrogen safety will also support the goals of DOE's FutureGen program.

Regional Collaborations

We are developing industry relationships as well as engaging regional and national interests in the creation of a Northwest Hydrogen Initiative. While this effort is just beginning, it will focus on developing a hydrogen infrastructure demonstration project, to characterize and communicate the societal benefits of a hydrogen economy, and to accelerate the development of national safety standards.
3.1.2 Vehicle Technologies:
Advanced Lightweight Materials
and Emission Aftertreatment

By building understanding of lightweight materials, including composites that could reduce vehicle weight by as much as 60 percent, and by developing exhaust aftertreatment technologies for diesel engines that could double the fuel efficiency in standard light-duty vehicles, PNNL is contributing to dramatic increases in vehicle fuel efficiency.

Our R&D efforts directly support EERE’s FreedomCAR and Vehicle Technologies Program. This program works in partnership with the domestic transportation industry, the energy supply industry, and R&D organizations to develop and promote user acceptance of advanced transportation vehicles and alternative fuel technologies. The primary goal for the FreedomCAR and Vehicle Technologies Program is to increase fuel efficiency to stop or reverse the annual upward trend in the quantity of petroleum fuels used by highway transportation vehicles. Secondary goals include reducing specific pollutant emissions and greenhouse gases and developing a strong transportation technology base that enables industry to ensure strong competition in the domestic and world markets.

Lightweight Materials

We are helping DOE achieve its goals related to transportation technology through our work in developing a new class of low-cost materials (e.g., thermoplastic composites, magnesium and titanium alloys), forming and joining technologies, and advanced computational design and manufacturing simulation tools to address key national technical needs for reducing vehicle weight and enabling the development of hydrogen powered fuel cell vehicles. We are collaborating with Oak Ridge National Laboratory on several of these efforts.

Through our CS&EI (Module 2.4.1) we have developed core capabilities in computational modeling of composite material systems that can use basic constitutive properties and processing knowledge to predict mechanical and thermal properties and, as such, enable the discovery of a new class of high-strength, low-weight materials.

Emissions Research

We are developing exhaust aftertreatment systems to control harmful pollutants in diesel exhaust emissions, providing a key enabling technology for widespread use of diesel engines in the United States. Diesel engines provide the best near-term approach to reduce U.S. petroleum consumption and reduce carbon emissions to the atmosphere. We are also applying capabilities in surface chemistry, catalyst mechanisms, models, material synthesis, and aerosols to build an understanding of
catalytic processes and advance the development of practical aftertreatment devices that can be commercialized for diesel engines. This area of research will also build on SC’s focus on catalysis and plans for a catalyst laboratory.

Our vision for the future is that we will have a laboratory for engine exhaust and emissions research (Module 3.7) that will provide capabilities for understanding phenomena in aftertreatment devices, experimentation and modeling focused on mesoscale aspects of emissions reduction technology, and rapid materials innovation. This facility would allow for an integrated approach that includes mechanism investigation, modeling, and materials/system optimization, leading to testing and validation.

The critical component of any engine emission device is the catalyst, so increasing our fundamental understanding of catalysts is imperative for advancing these technologies.

PNNL is developing exhaust aftertreatment systems that could enable widespread use of diesel engines. At this time, diesel particulate filters such as these are highly effective for pollution abatement, but are not sufficiently developed for widespread deployment.

3.1.3 Catalysis for Bio-Based Products and Fuels

PNL is developing methods for cost-effective conversion of complex biomass and synthesis gas into fuels for use in transportation and generation of electrical power.

Our chemical and biological capabilities enable us to develop breakthrough processes for bio-based products and fuels. These efforts support two key priorities of EERE—reducing the nation's requirements for imported petroleum and advancing the economic viability of a U.S. bioproducts industry. In addition, these capabilities are applied to produce higher-value chemical intermediates from synthesis gases, sugars, and oils. Our technologies are critical technical and financial components of DOE’s vision for an “integrated biorefinery of the future,” that complements ethanol production and creates a financially robust energy and bioproducts industry based upon renewable resources.

Innovative Catalysis Research for Products from DOE’s Sugars Platform

Building upon fundamental knowledge of catalytic processes and catalyst formulation, including advanced biocatalysis techniques, we are developing new processes to convert sugars and oils to chemical products. This research is needed to produce chemical building blocks used in industrial and consumer products while avoiding the use of petroleum and production of unwanted byproducts. This research also is expected to lead to new families of chemical intermediates for products with properties not currently available from the petrochemical industry, such as biodegradability, recyclability, and other desirable attributes.

For more than a decade, our unique catalysts and catalyst support systems have proven to be robust and efficient in the wet, condensed-phase conditions where biomass typically reacts. These catalytic systems provide both higher activities and longer lifetimes than catalysts previously available. Our unique laboratories and instruments that leverage support from EERE, including a new Symyx combinatorial chemistry workstation, are important components of this capability. To support the growth in bio-based products research, we are planning a Bioproducts, Sciences, and Engineering Laboratory (Module 3.7).

Improved Processes for Fuels and Hydrogen

We have spent more than 30 years developing chemistry and chemical engineering expertise that is critical to DOE’s biomass gasification and biopower program. We continue our contributions to the current synthesis gas program by developing and demonstrating innovative, breakthrough catalyst formulations and catalytic systems that significantly reduce the cost of producing bio-based fuels and chemical precursors using synthesis gas feedstocks. In particular, we are merging state-of-the-art technology in heterogeneous catalysis and micro-channel/micro-scale technology to provide the next generation of reactors for producing fuels from synthesis gases at a scale compatible with financially viable biomass operations. We are also using
our expertise in robust catalyst formulations to catalytically convert ligno-cellulosic biomass in aqueous solution, such as residues from dry-mill ethanol plants, to a methane-rich fuel gas. The technology also allows wastes such as bovine manure to be efficiently converted to energy products while alleviating environmental problems.

We are developing catalytic technologies that afford innovative, cost-effective routes to produce hydrogen from biomass, relying on signature strengths in catalysis and nanotechnology (Module 3.1.1). We are exploring how to convert biomass products (created as part of the sugars platform research) into hydrogen. These products serve as liquid hydrogen “carriers” that can safely and efficiently be transported to sites where hydrogen is needed. The catalytic reforming of these intermediate carrier products can generate hydrogen for a variety of uses. We also are examining basic biological pathways to create hydrogen directly from biomass resources through the use of microorganisms as even more efficient hydrogen production pathways for the future.

Chemicals and Products Research with Industry

We are a leading DOE laboratory for developing chemical intermediates and other industrial products in conjunction with industry partners via cost-shared projects enabled by Cooperative Research and Development Agreements. These projects focus on very early proof-of-concept research, rapid reduction of concept to practice, and clear demonstration of commercial viability for new technology. For example, our researchers, working in collaboration with Archer Daniels Midland and the National Corn Growers Association, developed processes that will reclaim greater value from the hull fiber that is removed from corn kernels during the first stages of corn milling and traditionally sold at cost as livestock feed. After less than two years of laboratory research, this process is now ready to be scaled up and will be demonstrated at the pilot scale during the next two years.

Scientists at PNNL used NMR spectrometry and other advanced technologies to determine the molecular components of corn fiber oil, an integral part of a joint research project with Archer Daniels Midland and the National Corn Growers Association. This team developed a new process to economically recover low-cost corn fiber and convert the carbohydrates and lipids from this fiber to ethanol, polyol chemicals, and specialty oils, plus a higher value livestock feed.

Program Support in Partnership with the National Bioenergy Center

PNNL is part of the National Bioenergy Center, which provides DOE with technical advice and program support to help guide planning and analysis efforts—such as the Office of the Biomass Program’s Multiyear Technical Plan, Annual Operating Plan, and others—for the next generation of biofuel and bioproducts technologies. The National Bioenergy Center includes the National Renewable Energy Laboratory, Oak Ridge National Laboratory, Idaho National Engineering and Environmental Laboratory, and Argonne National Laboratory.
3.1.3.1 Bio-Based Products Initiative: Capabilities and Partnerships for Bio-Based Research and Products Development

Using a fundamental understanding of materials and catalyst formulation, complemented by innovative applications of emerging methods in molecular biology, PNNL’s strong bio-based capabilities will uniquely serve the needs of the Office of Biomass Programs within EERE.

Through our Bio-Based Products Initiative, we are striving to integrate advanced chemical and biological science to establish a signature capability in developing these advanced processes for fuels and chemical intermediates.

Catalysis Capabilities

Building upon established capabilities in materials science and formulation of heterogeneous catalysts, PNNL is directing targeted capability-development investments to establish a fundamental understanding of the behavior of catalysts in aqueous conditions typical of biomass conversion reactions. Leveraging existing instruments for catalyst characterization and in situ evaluation of reaction kinetics, we have enabled the formulation of next-generation, robust and effective catalysts suitable for conditions associated with bio-based conversion processes. These conditions include condensed-phase, high-temperature, high-pressure, and extreme pH. In support of DOE program goals, we have successfully established a distinctive capability in formulating catalyst supports and catalyst materials to enable conversion of sugars, oils, and synthesis gases to fuels and chemicals.

Filamentous Fungi

In addition to chemical conversion processes, this initiative will establish us as a leader in discovery of novel filamentous fungi, as well as new molecular biology tools for “engineering” these organisms to enable specific biological processes. We apply methods such as proteomics and bio-informatics to unravel the genes associated with regulating optimal production characteristics, nutrient uptake, and protein expression and enzyme production.

Partnerships and Collaborations

Through the Bio-Based Products Initiative, we are forming relationships with institutions—such as major grower associations, commodity processing companies, and chemical and energy companies with a commitment to renewable products—that support the EERE objectives. These partnerships ensure a focus on well-
defined outcomes for our research, provide a mechanism for cost-shared technology development and demonstration, and facilitate transfer of successful technology from the Laboratory to commercial deployment in the private sector, a principal goal of the DOE Office of Biomass Programs. Partnerships with the National Corn Growers Association, as well as several state grower associations, have already resulted in successful projects to move discoveries from the laboratory to the pilot demonstration scale. In the future, these partnerships will facilitate complete commercialization of these processes.

We also partner with other research institutions, particularly universities and other federal laboratories, to expand the breadth and depth of capability available to DOE in the bio-based products field. We are part of the National Bioenergy Center, a collaboration of DOE laboratories in the biomass area, including the National Renewable Energy Laboratory, the Idaho National Engineering and Environmental Laboratory, Oak Ridge National Laboratory, and Argonne National Laboratory. Our growing partnership with Washington State University (WSU) has resulted in several collaborative research projects and will lead to construction of a new, state-of-the-art, multiuser Bioproducts, Sciences, and Engineering Laboratory at the WSU Tri-Cities campus, to be shared by PNNL and WSU researchers. Design and construction of this new laboratory will be funded by Washington State, with PNNL providing significant technical support throughout design and installation of key instrumentation (Module 3.7). This shared facility will dramatically enhance our ability, along with our partners, to conduct biomass conversion research, and will provide WSU with greatly expanded laboratory and teaching space, affording an opportunity to develop a new graduate program in bioproducts science and applied biotechnology at WSU.

Battelle, as operator of PNNL, places a priority upon bridging discoveries at the laboratory bench to commercial deployment of the technologies that can result from this research. With its many industrial partners, Battelle provides an important avenue for transferring technology from the laboratory to the commercial sector. Complete development of bio-based product technology has been the focus of significant investment by Battelle in recent years, and PNNL technology will continue to benefit from Battelle commercialization investment.

Examples of recent Bio-Based Products Initiative accomplishments:

- Receiving FY 2003 funding for a second phase of development to advance the corn fiber separation and conversion process (jointly developed by PNNL and Archer Daniels Midland) to a pilot-scale demonstration in conjunction with the National Corn Growers Association.

- Receiving capital funds to procure a custom-developed Symyx combinatorial chemistry system that will significantly enhance PNNL’s ability to develop and test new catalyst formulations for bio-based product development.

- Receipt of the Society of Industrial Microbiology’s Charles Porter Award by one of PNNL’s staff scientists who works in the growing area of bio-based products and who conducts research related to filamentous fungi.

The Bio-Based Products Initiative will focus its capabilities in fungal biotechnology to develop the next generation of biological catalysis technologies for producing industrial products in biorefineries.

**PNNL’s Buildings Program reduces the energy intensity of our nation’s buildings, while providing for the occupants’ security, health, and productivity.**

Our core DOE Buildings business includes energy codes and standards, operations and maintenance, market transformation, and technology demonstration and deployment. In addition to our ongoing support to EERE in these areas, we will broaden our contributions to include:

- R&D of organic light-emitting diode (OLED) technology, a component of solid-state lighting research
- Development of advanced building diagnostics and controls, a near-term to midterm effort to develop and apply technology to reduce the energy intensity of buildings and enable management of peak energy demand.

Achieving these two goals increases the S&T content of our EERE business and, in the case of OLED technology, enables us to apply our fundamental science expertise and capabilities to the development and application of a new lighting technology.

We have the capabilities and laboratory facilities necessary to lead development of the OLED technology component of EERE’s Solid-State Lighting Program, including materials design and synthesis, thin film deposition and modeling, and molecular structure testing. OLED technology has the potential to transform lighting practices in homes and buildings, and because of its distributed nature, could lead to a 50 percent reduction in energy used for lighting.

**Ongoing Projects**

In the area of Automated Building Diagnostics and Controls, we develop advanced technologies that enable real-time building and equipment condition monitoring. These technologies ensure cost-effective, energy-efficient building operation and maintenance that also minimizes environmental impacts and creates a secure, healthy, productive indoor environment. Our work in automated building diagnostics and controls builds on our long-standing competency in building operations, which has led to the deployment of technologies in both the public and commercial sectors and positions us to provide significant contributions in the future. Our latest activities focus on applications of wireless technology, development of low-cost sensors, and development and application of diagnostic tools that facilitate energy and environmental management of commercial and residential buildings.
We play a significant role in improving building energy efficiency by supporting stronger building energy codes, including their adoption, implementation, and enforcement, as well as market transformation and technology demonstration and deployment. Through the Building Energy Codes projects, we assist DOE in developing and applying new and enhanced building energy codes and building practices that enable the use of new energy-efficient technologies and practices. Similarly, through our Building Energy Code Implementation projects, we work on behalf of DOE with government agencies, state and local jurisdictions, national code organizations, and industry to encourage the construction and retrofit of energy-efficient buildings. And through our Market Transformation projects, we collaborate with DOE and industry partners to develop and implement programs to create and stimulate viable markets for new energy-efficient products.

Through this suite of projects, which includes technology demonstration and deployment, we help speed the adoption and implementation of building energy codes and the deployment of energy-efficient technologies to a wide range of customers and stakeholders including federal agencies, state and local governments, and international agencies.

PNNL is conducting thin film research to develop OLED technology in the pursuit of revolutionary low-cost, efficient lighting.
3.2 Supporting Electric Transmission and Distribution Reliability

As a major resource in the national effort to safely, efficiently, and reliably meet the electricity needs of the United States, PNNL is applying multidisciplinary capabilities to all aspects of the energy system, from generation to transmission, distribution, and end use of electricity.

We are supporting the newly created OETD in two primary areas—transmission reliability and electric distribution transformation. Aligned with this new office's goals, our research, development, and demonstration projects will enhance the electricity delivery system to ensure economic and national security. Our technical leadership in real-time systems analysis, large-scale power systems modeling, and advanced sensors is recognized by industry and valued by DOE. Combined with our understanding of competitive markets, regulatory frameworks, and demand response programs, we are creating a new paradigm that will transform the energy delivery infrastructure of the future.

Transmission Reliability

We are applying strengths in simulation, measurement, and analysis to help determine factors that may cause the national electrical transmission system to break down—and ensure the system does not reach those breaking points. Our transmission reliability research and technology development focuses on understanding and managing the behavior of the electrical system in the areas of automatic controls, system operations, and planning.

The DOE Transmission Reliability Program and the ongoing Wide Area Measurements System (WAMS) effort provide a general framework for these activities. This effort is specifically designed to meet the information needs of the changing power system, with a strong focus upon sharing federally owned knowledge and technology that is critical to ensuring reliability.

With support from the DOE Transmission Reliability Program, WAMS is now being extended into the Eastern Interconnection. The suite of measurement technologies and associated information analysis tools enables better decisions and insight into highly complex grid behavior that is undetectable with conventional technology. We will continue to address model validation and calibration as part of this program and its expansion to new regional transmission systems. In addition, we will continue to develop and analyze tools for grid management and conduct research related to demand response as a member of the Consortium for Electric Reliability Technology Solutions, in support of the DOE Transmission Reliability Program.

Electric Distribution Transformation

We support OETD with its program to develop a communications and controls environment that will enable transformational change in electric services. The inception of the program has been significantly influenced by PNNL's Energy Systems
Transformation Initiative (ESTI) efforts (Module 3.2.1). The program builds on internally funded research, and the resulting GridWise vision. In particular, using highly accessible telecommunications and information technology will enable value to be communicated transparently throughout the electric system. Better communication of value and data will facilitate participation of distributed energy resources (specifically distributed generation, storage, and load), permit active customer (and equipment) response and market participation, and enable more stable energy markets. Overall, the energy system will become more responsive, robust, secure, and reliable as a result.

Specific activities to support this transformation include assessing integration issues resulting from distributed energy resource technologies from multiple vendors in the distribution system and testing the technical and economic impacts of large numbers of these devices on the distribution system and transmission network. We also will explore the institutional, business, and policy issues associated with adopting advanced communications and controls systems. Architectures to empower all stakeholders (producers, consumers, distributors, and regulators) to respond to market prices and system constraints will be established through open communication and control architectures.

Our leadership in this program includes the following five areas:

- **Architecture** – Establish the technical and economic framework for a distributed electrical and business environment.
- **Applications** – Develop new functions and capabilities for the energy system through transformational technologies.
- **Simulation and Analysis** – Hypothesize, study, and predict the impacts of implementing transforming strategies and technologies that model physical, market, and regulatory aspects.
- **Test Beds and Demonstrations** – Gain insight into the issues and requirements of implementing transformational concepts and facilitate their early adoption.
- **Stakeholder Engagement** – Engage stakeholders in examination and advancement of transformational concepts to ensure all potentially affected or interested parties are informed and have the opportunity to participate.

These graphs show the difference between measured and simulated grid performance during the August 10, 1996, western grid breakup.
3.2.1 ESTI: Bringing the Electric Grid into the Information Age

PNRL’s vision of the energy system of the future includes creating a collaborative network embedded with real-time information and intelligence that integrates supply, demand, transmission, and distribution with new “plug-and-play” technologies, distributed generation, energy storage, and customer load management.

The ESTI is investing in research that will enable physical devices, commercial instruments, and public/private organizations to collaborate through advanced forms of information exchange, optimizing the energy system to address the economic, environmental, and national security needs of our society.

GridWise: A Vision for Future Energy Systems

While the term GridWise has been coined to represent a key ingredient of the intelligent grid of the future, the ESTI represents our internal investments in this area. We are developing industry relationships as well as engaging regional and national interests in the creation of the GridWise vision. The GridWise Alliance is being established to characterize and communicate the societal benefits of transforming the electric infrastructure, encourage interaction to develop synergistic commercial benefits, and accelerate the technical and regulatory transformations necessary to advance these concepts. This group includes industry leaders such as Sempra Energy Solutions, PJM Interconnection LLC, Alstom Esca Corporation, IBM Global Energy & Utilities Industry, and the Rockport Group, and indicates early support of our concepts by industry.

Our internal investments are building the basic long-term science foundation needed to support the transformation of the energy system, including capabilities in energy systems simulation, analysis, and controls. This work includes computer simulation tools that link economic market operations with the physical operation of the power system at both the retail/distribution and wholesale/transmission levels. Basic science is also being conducted to research new decision algorithms for analyzing optimal control of linked physical and economic systems, as well as a macro-level theory of transactive control that models the collective behavior of the vast numbers of interactions involved in such a complex system.

Technological Considerations

Our GridWise vision shapes a new era of energy commerce that allows transaction-based decisions to drive operations and planning at all levels of the system. The architecture to support the necessary communications reliably, securely, and with due consideration for privacy, must be scalable, resistant to failure and attack, and flexible enough to evolve as better technological solutions emerge. These requirements are not wholly unique to the energy industry, but are found in many sectors of commerce. This initiative foresees solutions that involve adapting and influencing mainstream information technology approaches to deliver an electric energy infrastructure in step with the architecture of the nation’s economy in general.
The crosscutting aspect of the initiative engages Laboratory-wide capabilities and creates opportunities for national and homeland security programs related to protecting the nation’s critical infrastructure. It also creates opportunities in other areas of DOE, including EERE, by looking at how fuel cells and other distributed resources can be integrated into the energy system of the future, and FE, with the potential for designing smart energy infrastructure that could affect fossil energy generation plants or account for carbon “trading” if that concept becomes a reality.

Examples of recent ESTI accomplishments:

• Providing the vision and leadership for a national program within DOE’s newly formed Office of Electric Transmission and Distribution.

• Maintaining two key advisory groups: the ESTI peer review committee and the CEO Coalition’s GridWise Alliance Board, which includes numerous industry leaders.

• Hosting the third Communications and Control Systems Distributed Energy Conference in 2002.

PNPL engineers are designing smart chips that can be fitted into household appliances to continually monitor the power grid for energy fluctuations. When the grid is under stress, a grid-friendly appliance would identify these fluctuations and, within milliseconds, automatically shut down for a short period of time to give operators time to stabilize the system.
3.3 Developing Clean and Efficient Fossil-Based Power and Hydrogen

PNL is developing innovative technologies that will support development of the world’s first fossil-fuel-based, pollution-free power plant and enable the transition to the hydrogen economy.

By 2015, FE is striving to design, construct, and operate a 275-megawatt prototype power plant that produces electricity and hydrogen with near-zero emissions. Virtually every aspect of this cutting-edge plant, known as FutureGen, will incorporate state-of-the-art technologies including fuel cells, hybrid energy systems, and techniques for coal gasification and carbon sequestration. Our R&D of fossil-based power and hydrogen generation systems will play a critical role in FutureGen and DOE’s vision to use existing supplies of fossil fuels in a cost-effective and efficient manner and with minimal environmental impacts. With capabilities in solid oxide fuel cell technology, materials science, surface chemistry, catalysis, electrochemistry, and carbon sequestration, we will help identify and address the technical barriers necessary for FutureGen to become a reality.

Solid Oxide Fuel Cells

As a leader in solid oxide fuel cell technologies, we are providing problem-solving research to optimize fuel cell systems and address the technical and economical challenges to commercialization of these systems for stationary, transportation, and military applications (Module 3.3.1). The modular fuel cells developed as part of SECA—managed by PNNL and the National Energy Technology Laboratory (NETL)—will become the basis of the FutureGen plant.

High-Temperature Electrochemistry Center

Through management of and participation in the High-Temperature Electrochemistry Center, we are collaborating with NETL and universities to provide crosscutting multidisciplinary research aimed at developing the advanced electrochemical technologies necessary to integrate the many components of FutureGen.

We conduct the majority of the center’s core research with emphasis on electric performance, thermoelectric materials, regenerative fuel cells, membranes, and sensors. In 2002, Montana State University was identified as a satellite research center with a focus on deposition of metal oxide thin films and electrical reactions at buried interfaces. Additional universities will be added as satellite centers focusing on specific topical areas or disciplines where new scientific knowledge and innovation are needed to support FutureGen. These university partnerships also create opportunities for student internships and visiting scientists—helping develop scientific resources for solving the energy generation challenges of the future.
Carbon Management

Our Carbon Management Initiative (Module 3.4) is focused on developing the science that will lead to technologies for capturing and sequestering carbon. These technologies will be coupled with new systems to generate energy and hydrogen as part of FutureGen. Building on capabilities derived from waste treatment activities at the Hanford Site, we are applying our geochemical expertise to build an understanding of how to capture and contain carbon dioxide and assess its effect on the surrounding geology and hydrology.

We have the lead for technical integration in the newly established Midwest Regional Carbon Partnership (RCP), located in the heart of U.S. coal country. The Midwest RCP is one of nine national partnerships.

PNNL’s participation in the High-Temperature Electrochemistry Center will help provide the technical underpinnings for fuel cell systems, turbines, and hybrid energy systems in support of developing large, land-based energy plants that are efficient, economical, and fuel flexible while producing near-zero emissions.
3.3.1 Advances in Solid Oxide Fuel Cell Technologies

Through its leadership in SECA and solid oxide fuel-cell R&D, PNNL will play a critical role in helping reduce the cost of modular solid oxide fuel cells for multiple applications to $400 per kilowatt by 2010.

SECA is a public-private alliance focused on making high-efficiency, low-cost fuel cells commercially available for a variety of applications. We jointly manage the alliance with NETL. Together, these laboratories coordinate solid oxide fuel-cell R&D to help FE achieve its mission to reduce dependence on imported oil and to mitigate environmental concerns associated with current methods of generating electricity from fossil fuels. We lead SECA’s Core Technology Program, which is focused on addressing technical barriers identified by the program’s industrial teams. Results from our research conducted as part of the Core Technology Program are shared with all the industrial teams to help advance their individual approaches to meeting the program’s overarching performance, size, and cost goals.

Our areas of research in support of the SECA program include materials and manufacturing, modeling and simulation, fuel reformation, and thermal management. We are well suited to tackle these technical challenges because we can assemble multidisciplinary teams with expertise in:

- analytical and physical chemistry
- chemical separations and conversion
- computational science and engineering
- design and manufacturing engineering
- electrochemistry
- energy technology and management
- materials S&T
- microengineering and nanoengineering.

Our researchers are developing computational models at the stack and systems levels that simulate operation of a total system, assisting in component design, studying schemes for fuel and oxygen delivery, optimizing plate configurations within a multiple stack, and building a better understanding of operating parameters. Based on a long history of materials research related to solid oxide fuel cells, our researchers also are improving electrolytes and electrical performance, developing new cathodes, increasing anode strength, advancing and improving seals, and minimizing thermal stress. In addition to reducing cost, this research will lead to increased efficiency, durability, and performance, as well as reduced start-up times.

SECA’s six industrial teams, including two new teams added in FY 2003, are pursuing a 2005 goal to develop 3 to 10 kilowatt solid oxide fuel-cell prototypes that would cost $800 per kilowatt when mass produced. By 2010, SECA targets $400 per kilowatt systems in commercial applications. These ambitious goals are aligned with FE’s FutureGen Initiative, a $10 billion effort to build by 2015 a next-
A generation power plant that operates on gasified coal and produces electricity and hydrogen while sequestering carbon for near-zero emissions (Module 3.4). Along with other SECA members, we will focus on developing large fuel cell clusters that use coal and coal gasification techniques to produce hydrogen and electricity in support of DOE’s FutureGen vision.

Solid oxide fuel cells that meet the size, performance, and cost targets of SECA are providing the building blocks for other national programs. EERE’s 21st Century Truck Program is focused on using fuel cells for auxiliary power systems and essential power systems in heavy trucks. The program concept adapts the SECA fuel cell for use on diesel-powered heavy vehicles. Using fuel cells to provide auxiliary power for heavy trucks instead of belt-driven generators powered by the engine will increase fuel efficiency and reduce emissions dramatically. Auxiliary power systems would eliminate the need for trucks to idle in order to maintain the necessary power for heating the diesel engine and sleeper cab and electronics.

The SECA fuel cell serves as the foundation for a program with NASA to adapt solid oxide fuel cells for aviation purposes. This program kicks off in FY 2003 and will first explore the use of solid oxide fuel cells for auxiliary power in commercial aircraft and may eventually consider their use for aircraft propulsion.

PNNL will build on its parent relationship with Battelle to bridge discoveries related to fuel cells to commercial deployment. For example, researchers at PNNL do some of the R&D for one of the SECA industrial teams—the Delphi-Battelle team. We have processes and procedures in place to ensure that any potential conflicts of interest are avoided and that DOE work receives first priority. At the same time, this relationship helps move technologies into the marketplace where they can begin making an impact in increasing efficiency and reducing emissions, consistent with DOE’s energy and technology transfer missions.

PNNL, through its leadership of SECA and the alliance’s Core Technology Program, is developing solid oxide fuel cells that can generate electricity from traditional fuels for a wide variety of applications.
3.4 Furthering Capabilities and Partnerships Through the Carbon Management Initiative

The Carbon Management Initiative seeks to establish PNNL as the DOE laboratory that has most profoundly shaped the nation’s approach to addressing climate change, while simultaneously developing new science and technology programs.

Signature Areas

To achieve our desired level of impact, we will emphasize three signature contributions:

1. Building the basic scientific understanding of climate change phenomena and ecosystem impacts.
2. Developing computational tools and techniques for evaluating alternative strategies for managing the potential risks of climate change.
3. Developing and deploying technological solutions to address climate change.

Tools and Techniques

Our investment in this signature area will focus primarily on delivering analytical tools that will provide valuable information to DOE’s newly created Climate Change Technology Program Office and its strategic planning process. This new office is intended to coordinate implementation of the President’s Climate Change Technology Initiative with the Department of Commerce, which coordinates the President’s Climate Change Science Initiative. By applying the integrated assessment modeling capabilities developed with support from SC to both presidential initiatives, we can be an analytical leader and profoundly increase our national impact. These efforts also will position PNNL’s Joint Global Change Research Institute, a collaboration with the University of Maryland, for expanded programmatic support. With increased support, the resources of the institute will become more widely available to support DOE’s needs.

The Carbon Management Initiative also supports the efforts of FE, which is looking toward carbon capture and sequestration technologies for its next-generation energy plants.

Technological Solutions

This third signature area will focus on carbon dioxide (CO$_2$) capture, sequestration, and monitoring and will receive the majority of the initiative’s investment, including nearly all capability-development investments.

In the area of CO$_2$ capture, we are focused on novel technologies that have the potential to separate CO$_2$ from power plant and industrial flue gases at a significantly lower cost than today’s amine-based systems. The use of nanomaterials offers exciting possibilities for novel separation processes due to the tremendous...
potential in preparing chemically selective solids with exceptionally high surface area. To be effective, however, there is a critical need to characterize the uptake of chemicals in such nanomaterials and to understand their chemical selectivity and other properties of interest for capturing CO$_2$. Targeting this area also allows the Carbon Management Initiative to leverage investments made by the Nanoscience and Technology Initiative (Module 2.5.3).

With respect to sequestration, we are examining geologic sequestration in three types of formations: deep-sedimentary, saline-filled formations; deep-basalt, saline-filled formations; and gas hydrate-bearing formations. Deep-sedimentary formations are the most prevalent in the United States and the likely choice for the nation’s first large-scale sequestration demonstration. Our work will develop a better understanding of the mixing behavior of supercritical CO$_2$ in brine-filled porous media and the long-term effects of exposure to high-pressure CO$_2$ on the physical, chemical, and mechanical properties of caprocks. We will also develop new capabilities for studying the behavior and effects of supercritical CO$_2$ in sedimentary rock formations.

While basalt formations are not as widely available, their geochemical composition offers the unique ability to mineralize CO$_2$ in situ, chemically trapping the CO$_2$ permanently. Building upon our extensive knowledge of Columbia Basin basalts, this work will determine the rate of CO$_2$ consumption by chemical reaction with selected basalt rocks under realistic conditions of pressure and temperature. Our goal is to better understand which primary minerals in the basalt react preferentially with dissolved CO$_2$ and to identify any surface-armoring reactions that could slow the kinetics of the mineralization process.

Permanent sequestration of CO$_2$ in methane hydrate-bearing formations while simultaneously producing methane offers a unique sequestration strategy that co-produces a valuable product. We will focus on understanding how a real gas injection and extraction process would or could work in porous media. To support this work, we have obtained natural hydrate-bearing core samples from the Canadian Arctic and from the Hydrate Ridge off the coast of Oregon. Researchers will characterize the physical and chemical properties of these samples through a combination of experimental measurements. We also will conduct injection dynamics experiments with these samples to ascertain the effectiveness of using CO$_2$ to dissociate the gas hydrate and recover the methane while permanently sequestering the injected CO$_2$ as a hydrate.

In the area of CO$_2$ monitoring, we are focused on novel, low-cost sensors and tracers that can be used to understand the fate of injected CO$_2$. The relatively high background levels of CO$_2$ in the atmosphere and soil, coupled with seasonal and diurnal variability, make it extremely difficult if not impossible to immediately detect small CO$_2$ leakage rates with existing technology. We will explore chemical and radiological tracers suitable for monitoring leakage of CO$_2$ from deep geologic formations. Two types of sensors will be developed for detecting the selected tracers: a laser photoacoustic spectroscopic sensor and a scintillating-grid radiometric gas sensor. The sensors will be evaluated for potential use in a future field demonstration.
3.5 An Integrated Approach to Nuclear S&T

We are integrating our nuclear S&T portfolio to address concerns related to national security, legacy environmental challenges, and options for energy generation that reduce both dependence on energy imports and greenhouse gas emissions.

For decades, DOE has been the center of the nation’s nuclear research and we have been a part of the R&D infrastructure that has enabled DOE to meet national needs related to nuclear energy, environmental management, international nuclear safety, and national defense and homeland security. With a long history of nuclear S&T expertise and a national reputation in radiation detection, nuclear fuels, and materials, our integrated nuclear strategy focuses on identifying areas of strength and enhancement needed to ensure that we can continue supporting DOE in the future.

National Defense and Homeland Security

Based on growing national needs, we anticipate significant programmatic growth in national defense and homeland security applications of our nuclear S&T capabilities (Modules 4.1–4.1.6). We also are making internal investments to establish Radiological Detection and Analysis Laboratories (RDAL) that will make these key capabilities more accessible (Module 3.5.1).

Advanced Energy Concepts

We intend to work with other laboratories to support DOE’s development of advanced reactors and fuel cycles, including playing a role in developing next-generation power reactors that are economic, safe, and proliferation-resistant, and are capable of becoming the base, advanced energy source to support a hydrogen economy. We will also focus on specialized energy sources, such as space power for national security, intelligence, and defense. While we do not expect significant near-term growth from NE, we will focus on maintaining our efforts related to space power, radioisotopes, the National Energy Research Initiative, and the International Nuclear Energy Research Initiative, as well as promoting nuclear education in support of our nuclear science and technology needs. These efforts are supported by our core capabilities in nuclear materials, including irradiation performance and structural performance, nuclear chemistry and advanced separations technology, and advanced diagnostics and prognostics.

Environmental Legacy

We apply our nuclear capabilities to provide cleanup solutions for areas contaminated during nuclear weapons production (Module 5.1).
Critical Capabilities

To make the nuclear S&T resources broadly valuable to DOE, we must recruit and retain critical staff in nuclear S&T and maintain specialized facilities and equipment. This includes replacing essential capabilities currently housed in facilities in the 300 Area. These capabilities will support expected radiological R&D involving ultralow-level through high-level radioactive materials (Modules 3.7 and 7.3).

As a result of the integrated nuclear strategy developed in FY 2003, we have a solid basis for managing staffing, facilities, programs, and S&T capabilities that support our customers:

- Office of Science (SC) (2.0)
- Intelligence (IN) (4.4)
- Office of Nuclear Energy, Science, and Technology
- Office of Environmental Management (EM) (5.0)
- Office of Civilian Radioactive Waste Management
- National Nuclear Security Administration (NNSA) (4.1)
- Department of Homeland Security (DHS) (4.5)
- Defense Threat Reduction Agency
- Defense Advanced Research Projects Agency
- NRC (3.6)
- U.S. Department of Defense (DoD) (4.6)

Taking an integrated approach to PNNL’s nuclear S&T enables us to leverage Laboratory capabilities across three major customer needs: legacy and environmental issues; national security interests related to nuclear, biological, and chemical weapons; and advanced energy systems.
3.5.1 Enhancing Nuclear S&T Capabilities

We are ensuring that our nuclear S&T capabilities are available to respond to the broad spectrum of needs identified by our customers.

Maintaining and enhancing our nuclear S&T capabilities, collaborations, and infrastructures are necessary to meet long-term needs for DOE’s related nuclear missions. We are committed to maintaining and adopting nuclear technical capabilities to address challenges in homeland security, legacy environmental issues, and energy production.

The focus of this crosscutting effort is on those areas that contribute most to DOE’s mission and laboratory vision. We intend to become the preferred source for radiological detection and analysis capabilities for the development, evaluation, and deployment of effective nuclear and radiological sensing instruments and systems to meet broad customer needs.

Establishing Radiological Detection and Analysis Laboratories

We perform R&D to provide novel technologies for rapid, automated trace detection and analysis of sensitive materials. By developing and integrating a suite of advanced capabilities in this area, our Radiological Detection and Analysis Laboratories (RDAL) will enhance our ability to provide radiological detection and analysis to many areas within DOE as well as other government agencies.

This effort will be structured to allow project managers to undertake interdisciplinary projects and use the diverse resources as needed to meet client project requirements. Overall, these laboratories will increase visibility and access for capabilities and will further strengthen capabilities by promoting teaming with universities, industry, and other government agencies. Collaborating with universities will enhance the supply of qualified staff in this area available to PNNL and other laboratories within the DOE complex.

Instrumentation capabilities within these laboratories can be deployed in interdisciplinary, multisensor systems, such as “portal measurement systems” to give enhanced border security and in meeting test and measurement needs to support programs in the National Nuclear Security Administration and Defense Programs.

Detecting and Preventing Nuclear Threats

In FY 2004 and beyond, new trace analytical capabilities will be developed to prevent and detect proliferation of weapons of mass destruction. Examples of internal research related to nuclear nonproliferation and attribution include a project for advanced and automated radiochemical analysis and another on electrode structures for high-pressure xenon detectors.
Building Radiochemical Processing Capability for Environmental Management

Advanced actinide separations technologies and the behavior of actinides in the environment are two areas of development. The benefits of advanced actinide separations technologies include reduced cleanup costs, reduced amounts of waste requiring disposal, and recycle of useful isotopes. Research challenges include aqueous separations for waste volume reduction and the transmutation of waste for nuclear reprocessing applications. These breakthroughs will accelerate the environmental cleanup of nuclear wastes at the Hanford Site and enable us to make contributions to waste cleanup and environmental restoration challenges worldwide, including the characterization of contaminated sites, monitoring of remediation and disposal facilities, and sensing technology for process monitoring and control.

Supporting Nuclear Energy Plants

This effort supports nuclear energy by developing S&T for the current and next-generation nuclear systems that would serve as a major power source to produce hydrogen along with clean fossil and renewable energy options. We are currently seeking knowledge in two areas that support the needs of the NRC: 1) the life-limiting degradation of light-water reactor materials and components and 2) the development of diagnostic and prognostic tools for advanced reactors (Module 3.6). These efforts will help extend the lives of reactors and improve operational effectiveness and safety.

Maintaining Critical Resources

The Laboratory is committed to building and sustaining critical capabilities needed to support DOE’s missions.

Continuing to make critical nuclear S&T resources available to DOE will require retaining and enhancing strong nuclear science and engineering capabilities. Establishing the RDAL, and coordinating this with a strengthening of our sensors and electronics capabilities, is an essential component in our facility strategy (Module 7.3).

Examples of recent nuclear S&T accomplishments:

- Refocusing FY 2003 efforts on the nuclear component of national and global security—areas where significant needs exist.
- Hosting the 40th DOE Weapons Agencies NDT Organization meeting, which resulted in proposals for target characterization studies to support the National Nuclear Security Administration and an invitation to participate in development of the Advanced Non-Destructive Engineering Strategy for the Nuclear Weapons Complex.
- Preparation of “Nuclear Technology Paths Towards Carbon-Free Energy” for publication; this led to a proposal to the Office of Nuclear Energy, S&T.
- Investigating the fundamental aspects of radiation-induced degradation of materials to support material evaluation needs for extending the licenses of power nuclear reactors.

We are building critical capabilities in nuclear S&T to solve problems in cleanup and national security.
3.6 Energy-Related R&D for Others

The energy-related R&D PNNL conducts for other government and private clients applies capabilities developed by DOE to solve national needs and enhances the resources and capabilities available to DOE in the future.

U.S. Nuclear Regulatory Commission

We fulfill DOE’s commitment to the NRC to provide world-class technical capabilities from the national laboratories in support of the NRC’s nuclear safety mission. Our work for the NRC addresses nuclear fuels, nuclear reactor pressure boundary materials, nuclear materials characterization, environmental transport of radionuclides, spent fuel storage and transportation, operating plant license extensions, nuclear facility safety, regulatory criteria development, and international regulatory program development. We provide NRC with internationally recognized experts in nuclear fuel burn-up and nondestructive examination analyses.

We support the three major divisions of the NRC:

- The Office of Nuclear Reactor and Regulation, which is responsible for ensuring public health and safety through licensing and inspection activities at all nuclear power reactor facilities in the United States.
- The Office of Nuclear Regulatory Research, which plans, recommends, and implements programs of nuclear regulatory research. We contribute our expertise in nondestructive evaluation of reactor vessel materials and in nuclear fuels performance assessments to meet this office’s needs.
- The Office of Nuclear Material Safety and Safeguards, which focuses on public health and safety through licensing, inspection, and environmental reviews for all activities regulated by the NRC except operating power and nonpower reactors.

Overall, our work for the NRC supports the continued operation of 103 nuclear plants that provide approximately 20 percent of the nation’s electricity—the equivalent of millions of barrels of oil.

National Aeronautics and Space Administration

From basic research to developing specific solutions relating to energy technologies, environmental technologies, and climate physics, we support NASA missions that relate closely to DOE mission areas. We intend to focus on the following areas of research and development for NASA:

- Developing new applications of microtechnology for NASA space missions including fuel production for Mars missions.
- Developing new nuclear space power systems.
- Developing fuel cell systems for commercial aircraft, in collaboration with NASA’s Glenn Research Center (Module 3.3.1.)
- Support for NASA’s Earth Science Enterprise in areas of climate and atmospheric chemistry modeling and in the application of NASA satellite instruments that support the ARM Program’s research objectives, which include research on clouds, aerosols, and climate; use of satellite-based remote sensing in climate research; and applications of remote sensing to natural resource assessment.

**Bonneville Power Administration**

Our strategic research with BPA regarding energy system reliability and environmental compliance has led to real-time grid monitoring that is integral to DOE’s new OETD (Module 3.2). Our environmental support includes fishery science that helps ensure sustainable operation of the hydropower system in the Pacific Northwest.

**Commercial Energy**

Our researchers apply their capabilities to commercial R&D for nongovernment clients in areas including nuclear materials safety, advanced clean power generation concepts, next-generation power systems, and low-emission vehicle technologies.

We work with automotive manufacturers and automotive equipment manufacturers to explore lightweight materials, exhaust aftertreatment technologies, and solid oxide fuel cells for use in auxiliary power systems for heavy trucks and aircraft.

In another example, we are supporting efforts to reduce energy use at the nation’s military bases by installing monitoring and diagnostic technologies as well as performing energy audits to determine opportunities for energy efficiency improvements.

These efforts help move government advances into real-world applications where they can benefit the environment, energy efficiency, and the nation’s economy. We also work with commercial firms to establish major public-private partnerships in DOE areas of interest such as carbon management and low-emission vehicles.

PNNL’s development of Decision Support for Operations and Maintenance, or DSOM®, and its use by the New York Housing Authority to reduce energy costs and maximize efficiency of its facilities is an example of how work for commercial customers supports DOE’s missions.
3.7 Infrastructure Needed to Support Energy Research

New facilities and investment in infrastructure are needed to support PNNL’s energy-related research, particularly to support research related to bio-based products, emissions and fuel efficiency, and nuclear S&T.

Bio-Based Processes and Products

We are teaming with WSU Tri-Cities to construct a Bioproducts, Sciences, and Engineering Laboratory. This facility will support rapid creation and deployment of new bio-based products that use agricultural byproducts and residues, supporting the regional agriculture economy and increasing the competitiveness of regional food processors while addressing national and regional energy needs (Module 3.1.3). This facility will consolidate our biomass research laboratories into a single space at approximately 60,000 to 70,000 square feet. Further, this modern laboratory will provide the ability to conduct research in both chemical and biological processes, supported by the best analytical and concentration and purification methods available. This showcase facility will support DOE research as well as draw industrial and academic users to collaborate with our scientists.

Nuclear S&T

Radiological and radiochemical facilities are essential to high-quality nuclear science and technology work. During this planning period we are readying our Radiochemistry Processing Laboratory for transfer to the site cleanup contractor, while continuing to use our unique capabilities to support national security, environmental management, and energy clients. Key to maintaining core radiological capabilities are the planned radioscience and global security buildings.

Increasing Fuel Efficiency and Reducing Emissions in Vehicles

In support of EERE and its goals to maximize fuel efficiency while minimizing harmful emissions from vehicles, we plan to consolidate its resources related to emissions research. By centralizing this equipment, including a new diesel engine for testing, we can enhance our ability to understand emissions behavior and explore technologies that reduce emissions without negatively affecting fuel efficiency.
Catalysis Research

To maximize the impact of the EMSL as a user facility and to further develop environmental, chemical, and physical sciences in support of DOE’s mission, we are exploring the feasibility of building a catalyst research facility (Module 3.1.2). This laboratory would build on existing strengths in oxide chemistry, computational chemistry, computational fluid dynamics, chemical physics, nanoscience, and heterogeneous catalysis to focus on discovery in catalysis and chemical transitions and expediting catalyst development and testing. While the primary intent of the facility is support research for BES, we also would leverage these capabilities to support the missions of EERE and FE.

Fuel Cells and High-Temperature Electrochemistry

Ongoing and expanding efforts to explore solid oxide fuel cells (Module 3.3.1), hydrogen energy systems (Module 3.1.1), and high-temperature electrochemistry (Module 3.1), will require a greater need for laboratory space with ventilated hoods. Because much of this work involves hydrogen and other flammable gases, these hoods are needed to conduct our materials development and cell testing. Larger, walk-in hoods, such as the two added in the HITEC Laboratory in FY 2003, allow more experiments to be conducted at the same time and more effective use of the equipment. In addition, limits on how much hydrogen can be stored inside a building led to the purchase of a hydrogen generator in FY 2003. As our programs continue to expand, there may a need for additional hydrogen generators.

The Bioproducts, Sciences, and Engineering Laboratory has received support from the state of Washington; the facility design costs are included in the state’s FY 2004 budget.
4—Security
4.0 National Security: DOE Mission and Strategic Intent

PNL will be a leader in national security and homeland defense, applying fundamental sciences to prevent the proliferation of weapons of mass destruction, ensure compliance with international arms control treaties, and protect the nation’s critical infrastructures.

The State of Security

In the broadest sense, the strategic objectives of homeland security are to prevent terrorist attacks within the United States, reduce the nation's vulnerability to terrorism, and minimize the damage and recover from attacks that do occur. With those goals in mind, we will concentrate our efforts toward developing and deploying technologies to counter terrorist threats. These efforts include growth in sensor technologies for the detection of chemical, biological, radiological, and nuclear threats (Module 4.2) as well as providing capabilities for protecting cyber and other critical infrastructures. We also will support the DHS and their mission to enhance the security, safety, and reliability of borders and surface transportation systems, and support development of technical standards from detection to assessment to operational requirements. Coupled with growth in the DHS area will be the opportunity for advanced collaboration with the intelligence community.

The Foundation for National Security S&T Breakthroughs

The foundation of our R&D program in support of DOE’s national security mission is through our Defense Nuclear Nonproliferation work, conducted primarily for DOE’s National Nuclear Security Administration (NNSA). The Defense Nuclear Nonproliferation mission is vital to the President's high-priority strategic objectives—such as the war on terror, national security, homeland security, and non-proliferation—and will remain so indefinitely. Congressional support for Defense Nuclear Nonproliferation, as reflected in significantly increased appropriations and authority, appears robust and on the rise, though with a few persistent concerns (e.g., percentage of spending in the United States versus Russia; open competition). Our nuclear scientists are leading design enhancements and providing technical oversight for the NNSA tritium production program, while expanding into challenges associated with our aging nuclear stockpile and measuring and detecting nuclear explosions.

Solving Real-World Issues

Significant challenges we are undertaking will help DOE expand its successful Materials Protection, Control, and Accounting (MPC&A) Program and International Nuclear Safety and Cooperation Program to other countries. Our core scientific capabilities have allowed us to expand our leadership role in growing NNSA programs related to radiological dispersal devices, reactor safety upgrades, weapons safety and security exchange, pit disassembly and conversion, and U.S. and Russian metal oxide fuel disposition.
Using PNNL's Capabilities to Counter Terrorism

Our Homeland Security Initiative is a prime example of how the Laboratory's broad scientific and technical capabilities provide value across all DOE mission areas. Working through the DHS's Science and Technology Directorate, we are focusing our technical expertise on developing and deploying the next generation of tools for early detection and prevention of terrorism. We are concentrating on sensors for weapons of mass destruction detection systems, information sciences related to protecting cyber and other critical infrastructures, and enhancing the security of our borders and surface transportation systems (Module 4.5). In support of our S&T agenda with DHS, our Homeland Security Initiative is pursuing a multiyear roadmap focused on technological advancements in detection of chemical, biological, radiological, and nuclear materials, and dynamic analysis of massive, diverse information streams (Module 4.5.1). Building on our homeland security capabilities, we will become a regional focal point of security technologies for the Pacific Northwest.

Discovering the Unexpected

Through our programs supporting DOE’s Office of Intelligence (IN), we are providing leadership in intelligence assessments surrounding the nuclear fuel cycle and nuclear weapons proliferation and non-nuclear energy security. Our Work for Others (WFO) Program is focused on intelligence analysis of all sources—nuclear, chemical, and biological—and includes information operations intelligence; methods development for integrating information, imagery, and multimedia sources; environmental forensics methodology development; infrared signatures applications; biometrics; small power sources; underground facility detection and characterization; and signatures intelligence in coastal regions (Module 4.6).

Supporting the U.S. Government

Basic and applied research projects within our National Security WFO Program are advancing our fundamental science capabilities in advanced materials and coatings, new sensors, biological and chemical detection and characterization tools, and molecular processes. Our clients include the Defense Advanced Research Projects Agency (DARPA) and the Defense Threat Reduction Agency, as well as the Air Force, Navy, and Army research laboratories (Module 4.6.1).

Our national security mission provides services to the Laboratory, the Hanford Site, and within DOE related to Safeguards and Security (Module 4.2) and Counterintelligence (CI, Module 4.3). Through our relationships with the Departments of State, Justice, and Treasury, we also bring reciprocal value to the Laboratory and DOE missions (Module 4.7).
4.0.1 National Security Mission Funding and Staff

The National Security Mission area will realize new growth in the intelligence and homeland security business areas.

The recently formed DHS is a significant new client for the Laboratory. New sales growth is expected, beginning in FY 2004, of approximately $50 million. Out-year growth could range from $100 to $150 million per year, contingent upon availability of staff and other resources.

Analytical technology products and R&D services for the U.S. intelligence community will result in 7 to 10 percent growth annually, over FY 2003 actual, reaching an estimated $70 million in revenue in 2010. By taking advantage of our core science and engineering capabilities, our all-source intelligence analyses, insightful scientific investigations, and innovative technology developments are recognized nationally as contributing solutions to gaps in critical national security challenges of concern to DOE’s Senior Intelligence Officer, the IN, NNSA, and the other 13 members of the intelligence community.

Some clear pathways for programmatic growth are:

- information sciences related to network forensics and development of network forensic information technology tools
- automated analysis of massive, dynamic data sets and streaming data; military electronics products across the spectrum of needs as utilized by intelligence and special operations forces
- a major DOE-based program for energy security related to non-nuclear energy intelligence
- advanced software systems for automatic registration and calibration of remote sensing imagery, including fusion of diverse image sources as unmanned aerial vehicles and satellite image sources
- specific contributions to radioisotope and conventional small power sources technologies, including continued development of methods for fabrication of extremely high-energy density batteries
- novel “smart” or “functional” materials that aid in fielding highly selective and accurate chemical, biological, and nuclear sensors and networks of sensors.

Major Programs Offset Flat Budgets

The DOE Office of Defense Nuclear Nonproliferation (DNN) business will remain flat to slightly declining, with reductions in the International Nuclear Safety Program. This decline, however, will be offset with growth in the MPC&A and Radiological Dispersal Devices (RDD) Program areas. DNN received $1.1 billion for FY 2003 as compared to $3 billion for the previous year, and has requested $1.3 billion for FY 2004. Along with these increased dollar amounts, Congress
recently provided DNN with future work for laboratory support, including authorities for the Elimination of Weapons-Grade Plutonium Program, MPC&A activities outside the former Soviet Union, and international nuclear safety and security cooperation activities worldwide. In addition, DNN appears interested in leveraging additional funds for such programs by implementing recently legislated authority to exchange Russian debt for Russian investment in nonproliferation activities.

**Supporting U.S. Armed Forces**

Prospects for the DoD business area are stable, but with growth sufficient to offset inflation. Due to the present funding shift to operations from development, DoD business is expecting moderate near-term growth. In the mid-term, transformation and reorganization activities are expected to create strong growth opportunities across our DoD portfolio. Good near-term growth is anticipated in the basic and applied R&D area, driven by long-range needs for new weapons detection technologies, advanced materials, and interest in nanotechnology applications. Moderate growth is expected in the environmental and energy sectors of our DoD clients, driven by regional management issues, range remediation, and base energy efficiency needs. Dramatic growth potential exists in advanced power systems, including fuel cells, small nuclear systems, and advanced solar technology. Defense systems work is fairly flat despite strong growth in logistics systems, as some older long-term programs have ended. Programs related to military applications have the same present trend driven by a switch of funding from development to operations. However, the R&D needs of transformation to a new type of military are starting to impact DoD R&D agendas; strong growth is expected in that area in the next few years.

![PNNL National Security mission area funding profile. Declines are projected as funding source changes to DHS.](image-url)
4.1 Defense Nuclear Nonproliferation Program

PNL is leading the application of fundamental science, environmental, and energy capabilities to critical U.S. national security challenges of detecting and preventing proliferation of weapons of mass destruction.

Partnering for Peace

Through NNSA sponsorship as well as nongovernment organizations, nonprofit foundations, conferences, and other private venues, we significantly contribute to furthering the nation’s goals related to nonproliferation and weapons of mass destruction. Our Defense Nuclear Nonproliferation Program will continue using traditional and nontraditional means to apply its strong S&T base to resolving international nonproliferation problems.

Our scientists and engineers provide leadership in nonproliferation research and engineering, particularly in the area of environmental sensor development for detecting proliferation of weapons. Our core competency in environmental monitoring is now being directed toward nonproliferation and environmental restoration involving development of technologies to monitor and measure all aspects of the plutonium pathway as it relates to nuclear weapons development.

Reactor Safety

We are carrying out nuclear safety improvements worldwide that reduce risks of terrorism directed against nuclear plants, stimulate the economy of emerging democratic nations, and stabilize host governments. This work contributes to fulfillment of a major international commitment of the United States. Using lessons learned from the successful reactor safety program in the former Soviet Union, we will expand nuclear safety activities into other nations whose nuclear production capabilities are of national security concern.

Warhead Dismantlement

We provide leadership in nonproliferation and international security S&T, particularly in the area of warhead safety and security and international nuclear fuel cycle projects. Through the Weapons Safety and Security Exchange program, we will continue to provide technical leadership in the areas of non-nuclear signatures, information barriers, tags and seals, emergency response, and adaptation of nuclear detection systems to antiterrorism applications. Through partnerships with universities and other laboratories, we will continue to develop new technologies to address treaty verification and transparency (i.e., ensuring that the United States and former Soviet Union nations each have access to the same information about each other for materials under treaty jurisdiction), export control concerns, and arms control verification issues.

S&T Transfer

We provide leadership in international nuclear MPC&A. We will continue to excel at transferring S&T to foreign entities in the areas of material inspection and oversight, training for safeguarding of nuclear facilities, and enhanced regulatory control
of nuclear materials. In particular, we will provide leadership in the development of detection and protection technologies for radioactive materials that could be used for radiation dispersal devices.

**Fissile Materials Disposition**

We provide significant contributions to fissile materials disposition activities related to plutonium materials. We will provide technical support for the Pit Disassembly and Conversion project through final design and construction. This project involves a unique, first-of-a-kind facility in this country for processing the pit of a nuclear weapon at DOE’s Savannah River Site to recover the plutonium for final disposition in the mixed oxide fuel facility. In addition, we will partner with other organizations to address technical issues associated with U.S. and Russian mixed oxide fuel facilities, help develop a strong regulatory framework under which to carry out fissile materials disposition activities, and continue to lead the formulation of international technical agreements associated with plutonium disposition.

**Infrastructure Needs**

Our leadership role in support of the nuclear nonproliferation mission relies, in part, upon critical infrastructure resources, including a number of radiochemistry facilities and specialized radiation detection and analysis equipment and instrumentation. Our plan for modernizing the PNNL research campus includes two new facilities with state-of-the-art radiochemistry, detection, and analysis capabilities.

Sponsored by DOE’s Office of Nonproliferation Research and Engineering, PNNL has developed a highly portable detector using neutron-sensitive scintillating glass fibers. These new detectors can be easily transported by a single person and rapidly deployed to establish a radiation detection capability for nuclear materials and radiological weapons of mass destruction. The ease of use allows simple and fast establishment of detection perimeters around special events at short notice.
4.1.1 Nonproliferation Research and Engineering

PNL’s unique perspective on the “plutonium pathway” will help DOE detect and prevent the proliferation of weapons of mass destruction.

Laboratory Investments Lead to New Opportunities

Our initiatives in infrared sensors, nanotechnology, and nuclear, biological, and computational sciences are providing critical new capabilities to address challenging nonproliferation needs. These investments are a critical element of the nonproliferation research and engineering growth strategy. Returns from investments in the infrared sensor initiative have resulted in a major new program (Remote Spectroscopy); exploiting the capabilities developed through the now completed Imaging Science and Technology Initiative is a key element of the nonproliferation research and engineering growth strategy.

The Next Generation of Scientists and Engineers

We are partnering with regional universities, such as the University of Washington, to address critical S&T requirements for national security. In addition, working with the universities is critical to developing the next generation of policymakers, scientists, and engineers to work on national security problems and in offsetting the “graying of the workforce” by bringing in new capabilities, insights, and enthusiasm to meet future U.S. nonproliferation needs.

Drawing Upon the Hanford Legacy

Our contributions to resolving Hanford Site legacy issues provide a unique perspective with respect to the plutonium pathway. Plutonium production processes—including fuel fabrication, reactor technology, reprocessing, metal production, and component fabrication—are critical steps in the weapons development pathway and represent the historical mission of the Hanford Site. The legacy of this mission and knowledge of the plutonium production process and signatures is critical to U.S. nonproliferation efforts, as it provides the definitive model for plutonium pathway to nuclear weapons development.

Our core competency in environmental monitoring, a direct outgrowth of the plutonium production mission, is now being directed at nonproliferation and environmental restoration. Expertise in monitoring nuclear processes, developed as part of the Laboratory’s plutonium production responsibilities, remains one of our longest standing missions and core competencies. This expertise is brought together to provide an integrated approach for sample collection and analysis, which is based on modeling, sample collection, preconcentration, separations, ultrasensitive measurements, and interpretation of results.
All of the Signal All of the Time (ASAT) is a focal plane detector that can detect and measure a broad range of ion masses simultaneously and rapidly from a small sample. The first significant advance in mass spectrometry detector technology in several decades, the ASAT detector maximizes data retrieval and efficiency. While traditional mass spectrometers provide a keyhole view of a small portion of the spectrum, the ASAT detector opens the door to the entire spectrum.
4.1.2 Nuclear Safety Cooperation Program

By extending its international nuclear safety expertise to a broad worldwide arena, PNNL is furthering the nation’s national security goals.

Eliminating Consequences of Terrorist Attacks

Enhanced nuclear power plant safety is reducing the potential for significant consequences from terrorist attacks at nuclear plants, promoting international business development and stimulating local economies, supporting global environmental goals, and helping stabilize host governments. Our researchers are making significant contributions to this effort by developing nuclear power plant safety improvements that directly reduce the risk of significant consequences from a terrorist attack.

Robust safety systems that incorporate state-of-the-art nuclear S&T ensure that an act of terrorism will have minimal impact on a reactor. A key to building a strong, stable, market-based economy is the establishment of a secure business climate. A nuclear power plant with questionable safety risks discourages international investment, thereby slowing the growth into a free market economy for a young democratic nation. The link between economic development and nuclear safety can be shown by the European Union’s demand that every former Soviet Union nation operating a nuclear power plant close their unsafe reactors before being allowed to join the European Union.

Nuclear power is a viable large-scale power source that can meet growing energy demands while supporting antipollution goals. However, a major nuclear accident anywhere in the world would affect the future viability of nuclear power everywhere, potentially eliminating this practical solution to one of the earth’s most challenging environmental problems. Political analysts cite the Chornobyl crisis as a key destabilizing factor that helped lead to the collapse of the former Soviet Union. A severe nuclear accident anywhere could destabilize the affected country and the surrounding region, causing severe human and economic suffering, just as in Ukraine.

In most countries with growing nuclear power programs, the organizations and professionals that support nuclear power are the same ones who develop nuclear weapons programs. To take advantage of the close organizational, personal, and professional links between nuclear power and nuclear weapons development in most nations, we are establishing a dialogue on nuclear power plant safety that is opening the door for cooperation on nonproliferation activities. The resulting relationships developed within a country’s nuclear power infrastructure will enhance our ability to monitor weapons development activities and to influence nonproliferation issues.
Applying Lessons Learned Worldwide

Engagement in nuclear power safety in many regions is vital to the our national security interests because of the presence in those regions of large, unsophisticated nuclear power programs, proliferation threats, and regional instabilities. We are addressing this need by making available to Asian nations the lessons learned from our highly successful reactor safety program in the former Soviet Union (see the figure). In addition to the ongoing work in the former Soviet Union, expansion of nuclear safety activities into China, Pakistan, India, and other nuclear-capable nations will help further the antiterrorism, foreign policy, environmental, and nonproliferation goals set by the United States. These nations must be provided modern nuclear S&T solutions to address the critical problem of nuclear facility safety to ensure that a global nuclear accident never occurs again.

At reactors in Russia and Ukraine, the frequency of minor safety events—a precursor to nuclear accidents—has declined sharply since DOE and PNNL began upgrading nuclear safety in these countries in 1992.
4.1.3 Nonproliferation and International Security S&T Program

By leading the assessment of technical policy options in a wide variety of nonproliferation and arms control problems, PNNL is enhancing global security.

Promoting Safe and Secure Storage of Nuclear Materials

Strengthening international nuclear safeguards is one of DOE’s critical program priorities. We provide leadership for international nuclear fuel cycle projects such as the canning and movement of BN-350 reactor spent fuel in Kazakhstan, and the canning and possible disposition of damaged North Korean spent fuel. We are also promoting solutions for maintaining weapons-usable nuclear materials in safe and secure locations, out of reach of possible terrorists or rogue states. Our extensive experience in nuclear materials production, handling, storage, and disposition is being applied to this effort. Application of innovative technical solutions to emerging problems, such as illicit trafficking of nuclear materials and regional security concerns, is contributing to the prevention of proliferation of nuclear weapons.

Solutions Intersecting Policy and Technology

Through contributions to the nuclear Warhead Safety and Security Exchange program, we provide technical leadership in the areas of non-nuclear signatures, information barriers, tags and seals, emergency response, and adaptation of nuclear detection systems to antiterrorism applications. We are building on our partnerships with universities and other laboratories to develop new ideas for verification and transparency while protecting sensitive information.

Science Contributes Solutions to Export Control Problems

The technological capabilities we used in developing nuclear and dual-use export controls are also applicable to export control problems involving chemical and biological proliferation. Work is continuing on expansion of capabilities to prevent proliferation of weapons of mass destruction. On behalf of our government clients, we are engaging in training and capacity building of export control officials worldwide.

Helping Weapons Inspectors Around the Globe

We are providing leadership to important programs of the International Atomic Energy Agency (IAEA), including ongoing programs in Iraq. Our staff are using their experience in nuclear material management and computer applications to continue to develop technological solutions to the problems of an expanding IAEA mandate and a growing international safeguards environment.
Putting Scientific Skills to New Uses

Our scientists are helping economic diversification in the nuclear cities of Russia through the Russian Transition Initiatives program. In one part of this program, former Soviet biological warfare scientists have switched to producing commercial agriculture and pharmaceutical products. We will expand our support of economic diversification by engaging additional scientists who are looking for alternatives to the design and production of weapons of mass destruction.

The Warhead Safety and Security Exchange program at PNNL promotes the exchange of unclassified technical information relating to the safety and security of nuclear warheads and their components during dismantlement, as well as technical information relating to nuclear and radiological counterterrorism. The exchanges under this program strengthen global security by reducing nuclear threats and fostering U.S.-Russian cooperation.
4.1.4 International Nuclear Material Protection, Control, and Accounting Program

Through its management of infrastructure and security projects, PNNL will help DOE develop and implement a strategy encompassing a broad range of activities to ensure the protection of nuclear materials worldwide.

Material Protection, Control, and Accounting

We are applying 50 years of nuclear materials handling experience at the Hanford Site to the challenges created by the nation’s heightened concern for terrorism, especially to the potential diversion of weapons-usable nuclear materials. Our innovative thinking and agenda-setting leadership will help ensure international protection, control, and accountability of nuclear materials. In addition, our world-class staff, fundamental S&T capabilities, and facilities are providing a wide range of technical expertise to the safeguarding and protection of nuclear materials in Russia, including physical protection, protective force, and material control and accounting upgrades.

Training the Trainers

We are leading the development of training activities for safeguarding and protecting nuclear facilities in Russia. Building upon our development of training related to the Russian Methodological and Training Center for Material Control and Accounting, and the Interdepartmental Special Training Center for Physical Protection, we provide regional and distance learning capabilities to the Russian nuclear materials complex. Our goal is to create Russian training programs that are robust and self-sustaining.

Developing Inspection Oversight Systems

We are assisting the Russian nuclear regulatory authorities in the development of an enhanced inspection oversight system. Russia also is being assisted in its development of a comprehensive regulatory system, relying on rule of law, and with adequate enforcement capability to ensure that the advances the nation has achieved in material control and accounting and physical protection will be bolstered by an improved, robust regulatory structure. Our contributions to the program include computer systems development skills, project management skills, and extensive regulatory development experience.
Leadership Management

We are training MPC&A program managers in management concepts and principles. Building upon our strength in integration and project management, we will continue to provide expertise to help DOE clients enhance their management of the complex programs of MPC&A, Second Line of Defense, and radiation dispersal device (RDD) protection and consolidation, as a closely coordinated, effective set of nonproliferation programs.

Detecting Radiation Dispersal Devices

We are helping DOE clients integrate and implement a worldwide program to limit the risk of terrorists developing RDDs. Assistance includes applying of S&T to the detection and protection of radioactive materials that could be used for RDDs, and providing expertise to national and international standards development organizations. We manage the development of guidelines to limit the risk of development of RDDs through establishing priorities and methods for protecting and eliminating the hazards of orphaned radioactive materials.

With the Institute of Physics and Power Engineering in Obninsk, PNNL is helping Russia develop the infrastructure to manage its nuclear materials.
4.1.5 Nuclear Nonproliferation’s Fissile Materials Disposition Program

PNNL’s core capabilities in nuclear science and engineering, process technology, policy and regulatory analyses, and nonproliferation and arms control will enable execution of critical U.S.-Russia plutonium management and disposition agreements in the coming decade.

Treaty Verification

Our technical expertise in process technology, nuclear science and engineering, and nonproliferation and arms control enables us to lead the development of strategies and provide technological solutions to ensure that high-profile international agreements on plutonium disposition will be met. We are the lead author on a multilaboratory paper that outlines how the U.S. government will verify the disposition of 34 metric tons of weapons-grade plutonium in Russia. Similar technologies will have to be deployed in the U.S. plutonium disposition facility. We will support DOE and other government agencies to obtain agreement on the technical approaches for these verification activities. We will lead the development of a suite of technologies that can make the needed measurements—providing life-cycle support from final development to field deployment.

Critical Partnerships

We will provide innovative and flexible approaches in supporting the fissile materials disposition mission via key partnerships with the private sector (primarily architect/engineering firms) and other national laboratories. An example is the partnership with Washington Group International on the Pit Disassembly and Conversion Project. We will continue to provide technical support to the design of this project through final design and construction, including support to the technology maturity evaluations of the Pit Disassembly and Conversion Facility (see the figure) design and providing additional technical support to address maturity issues or gaps in the technology. We will partner with other organizations to address technical issues associated with processing the diverse feed streams scheduled for mixed oxide fuel facilities here and in Russia. We will continue to use our process expertise to identify technology options for waste streams that are not candidates for mixed oxide fuel processing, but that require final disposition.

Regulatory Support

Through our expertise in policy and regulation analysis and nonproliferation and arms control, we are leading joint work with other national laboratories, DOE, NRC, and critical Russian organizations to successfully execute plutonium management and disposition agreements. With the declining infrastructure in Russia and the
need to construct and operate new nuclear facilities to meet the disposition agreements, there is concern related to the environmental, safety, and health regulations that apply or will apply to construction and operation of these facilities. Building on extensive experience with NRC and the safe operation of nuclear facilities in the United States, we will assist DOE with developing the regulatory framework for safe and efficient operation of these facilities, thus ensuring mission success while minimizing additional expense.

In partnership with Washington Group International, PNNL is providing expertise in criticality safety, process chemistry, and nuclear design for the Pit Disassembly and Conversion Facility.
4.1.6 NNSA Office of Defense Programs

We expect future roles in the DOE Defense Program stockpile stewardship mission building on our proven leadership in tritium production and our ability to apply our nuclear capabilities to ensure the safety and reliability of the nation’s nuclear weapons stockpile.

Tritium Production Leadership

Building on the success of the tritium production development program, we will continue to provide technical leadership expertise to the program. We will seek to retain the role of design authority for DOE and provide technical oversight for the production program. We will continue to provide design enhancements that reduce costs or improve production of this strategic nuclear material.

Defense Complex Partnerships

We are establishing partnerships within the defense complex to provide technology solutions to problems associated with the need to inspect, test, and certify the aging nuclear weapons stockpile. With the need to continue to certify the stockpile, the aging workforce and infrastructure is a significant DOE Office of Defense Programs (DP) issue. We will team with the defense complex management and operations contractors to provide technologies for inspecting or analyzing weapons and weapons components to assist with the stockpile certification, thus filling gaps created by the loss of critical resources during the past decade.

Weapons Stockpile Outlook

As DOE manages the nation’s aging weapons stockpile, needs may be identified for unique materials or for test monitoring and measurement. We have technological expertise that is well positioned for responding to future DP missions.

Infrastructure Needs

We have been working with DOE on a facility strategy that supports Hanford Site cleanup, maintains the Laboratory’s needed radiochemical processing capabilities, and provides the blueprint for our research campus of the future. Examples of the relevance of this effort to our DP work include the following:

- We are currently the technology arm of the Tritium Readiness campaign for DP. We perform all testing on tritium-containing, high-gamma dose materials. This is unique in the DOE complex, as most tritium handling is performed in glove boxes, and most high-level facilities do not handle tritium. With first-of-a-kind production starting this year, it is reasonable to expect some need for testing, particularly since the Tritium Extraction Facility will not begin operating before 2008. This facility is not designed for R&D work, and cannot handle individual tritium rods for examination. If this function is needed, this capability will have
to be maintained or created somewhere at considerable cost to the government. DP is also maintaining the ability to return to testing if so directed by the President. Our considerable expertise with environmental monitoring and trace radiochemical analytical work is directly relevant to this new mission. These capabilities, which we are proposing to maintain in our facility strategy to support other missions, would be available to support testing if needed.

World-class capabilities in nuclear design and materials and process development resulted in the successful deployment of the Tritium-Producing Burnable Absorber Rod.
4.2 Safeguarding and Securing National Security Assets and Government Resources

PNL topical area expertise in safeguards and security and core technical capabilities in nuclear science and engineering, environmental sciences, and large-scale information integration and management technology will enable the Office of Security to solve national security challenges related to threat identification and mitigation measures for special materials and critical information.

Improving the Reliability and Effectiveness of Threat Identification

Our ability to integrate vulnerability methodologies and technologies will improve the reliability and effectiveness of threat identification and assets characterization to prevent theft of materials associated with weapons of mass destruction and radiological and/or toxicological sabotage. With our extensive domain expertise, we will provide leadership in computer systems design and project management to develop robust systems approaches to emerging threat scenarios.

Securing Our Critical Infrastructures and Information

We will continue to provide innovative technology solutions for improved and efficient information security and physical protection measures of critical national assets. Building on demonstrated technologies and strong initiatives in infrared sensors and imaging S&T, we will promote solutions to labor-intensive protection measures. Cost-effective technological solutions for maintaining information integrity and asset protection will meet national and international objectives in the changing world.

We will continue to advance state-of-the-art technologies for collection, protection, and use of information critical to the DOE Office of Security mission. We will deploy our expertise in collecting and managing extremely large data sets to provide an integrated approach to the use of readily available information that currently represents an untapped resource. Resulting data will be analyzed to address difficult problems related to policy development and technology deployment.

World Leaders in Training Programs

We are providing topical area expertise in the management, control, and accounting of nuclear materials through successful training, policy analysis, technology, and site assistance programs. Our highly regarded international and domestic control and accountability training development experience will enhance domestic program effectiveness. Our core competency in environmental monitoring will be directed toward detection and monitoring movements of nuclear material through operating facilities or attempts at removal.
Developed by researchers at PNNL, optically stimulated luminescence-based radiation detectors can be used to detect special nuclear materials being smuggled into the country via sea containers. Also known as “smart sensors,” these battery-operated detectors are strategically located inside sea containers and information is collected via wireless personal digital assistants.
4.3 Office of Counterintelligence Support

PNL will develop an effective counterintelligence program that provides demonstrable value to the strategic missions of DOE, NNSA, and the U.S. intelligence community.

Protecting Freedom

The objective of the DOE national counterintelligence mission is to protect DOE personnel, assets, and programs from hostile foreign intelligence collection, espionage, and international terrorist activities. In support of these goals, we draw from our diverse resources to identify, assess, and neutralize hostile foreign intelligence services and terrorist organizations that are targeting national interests. The following three strategic goals have been defined as essential to the counterintelligence mission:

- Identify hostile foreign intelligence collection and international terrorist activities to address their respective threats against Laboratory staff and programs.
- Identify and eliminate risks of espionage (both traditional and economic).
- Educate staff to recognize hostile foreign intelligence collection and terrorist activities.

It is fundamental to the success of this program that measures be developed and deployed to safeguard DOE classified and sensitive programs, personnel, information, and critical assets from such hostile activities, and that trusted insiders acting on behalf of a foreign intelligence service or terrorist organization be detected and deterred.

A Three-Tiered Approach

Our counterintelligence program uses three distinct organizational elements to execute its commitment in support of DOE’s counterintelligence effort. One element consists of an operational group whose primary function is to perform essential counterintelligence responsibilities included in our contract with DOE. A second element consists of nationally based projects that support counterintelligence, specifically, the Inquiry Management and Analysis Capability and its Operational Analysis Center, which provides operational analysis of cyber threats across the DOE complex. The third element within our counterintelligence program provides special support to the DOE Polygraph and Inspection Programs. These three elements are fully funded by the Office of Counterintelligence; their combined annual budget is approximately $15 million. In keeping with national goals to grow a “workforce of excellence,” we will continue to staff these activities with highly qualified professionals empowered with up-to-date knowledge and state-of-the-art tools to ensure that the program maintains a focus on the future.
Collectively, this program will meet its strategic objectives by performing counterintelligence investigations, assessments, awareness training, and analysis. We will continue to explore every opportunity for collaboration across the DOE complex and with other agencies in the intelligence community to maximize the success of the program. Further, the counterintelligence program staff realize that trust, confidence, and mutual commitment from all Laboratory staff are vital ingredients in fulfilling these objectives. Consequently, program operational activities emphasize development of effective program awareness initiatives that will result in timely and issue-relevant incident reporting.

**New Analytical Processes**

Our counterintelligence elements will continue to develop technologies and implement new analytical processes that will aid the DOE complex in the formulation of timely and effective counterintelligence measures. Capitalizing on our experience in supporting the development of the DOE Information and Special Technology Program and Polygraph and Inspection Programs, these activities will be especially directed into the areas of information systems and personnel and program assessments. Advanced analysis capabilities and anomaly detection, particularly with respect to counterterrorism support, emerging cyber threats, homeland security, and critical technology identification, will continue to be priority areas of attention.

We also will regularly provide specially tailored counterintelligence analysis products to DOE and the intelligence community. In preparing these deliverables, our counterintelligence staff will be forward-looking, flexible, and responsive to changing threats. Counterintelligence staff conducting such research will exploit a number of strategic advantages to accomplish their objectives. They will use a wide variety of classified and unclassified databases and systems and work closely with our Field Intelligence Element and Safeguards and Security Services. Through these partnerships and proven capabilities, our counterintelligence program will have access to some of our nation’s most advanced intelligence information systems, visualization software, and network intrusion technology.  

An effective counterintelligence program leverages the full technical and intellectual capital available at the Laboratory, such as the Operational Analysis Center, which conducts network traffic analysis across the DOE complex. This center capitalizes on technical and analytical expertise from six technical groups across three PNNL directorates.
4.4 Intelligence Mission

PNNL’s all-source intelligence analyses, insightful scientific investigations, and innovative technologies will continue to contribute solutions to gaps in critical national security challenges for DOE’s IN, NNSA, and the other 13 members of the intelligence community.

DOE’s IN, NNSA, and the other 13 members of U.S. intelligence community have growing and urgent needs for all-source technical intelligence analyses and information science tools for analysis, specialized scientific investigations, and a variety of innovative technologies. Our unique capabilities in selected topical areas will contribute to meeting client needs in these and other areas.

Focus On All-Source Analyses

We will broaden our contributions to all-source intelligence analyses. Our core areas of analytical expertise include the nuclear fuel cycle, non-nuclear energy security, and information operations of intelligence interest.

Nuclear Fuel Cycle Assessments

With expertise in nuclear science and engineering, we will continue to fulfill our role as the leading technical analytical group for IN and others for intelligence assessments surrounding the nuclear fuel cycle and associated nuclear weapons proliferation. We are the principal provider of highly technical intelligence assessments for nonweapons intelligence issues; we plan to expand our leadership role with the IN and other federal agencies as the primary expert for such matters.

Information Operations Intelligence

During the past three years, we have expanded our intelligence analysis capabilities to meet the challenges of information networks and related network forensic issues for classified and unclassified sources. Our depth of skills in information S&T has enabled a natural transition from developing information technology tools to applying these and other tools to challenging information operations problems. Building on the success of this capability, three small analytical groups have been established with various agencies in and around Washington, D.C., where massive data visualization tools are being integrated into analytical working groups dealing with intelligence analysis in information operations. We are positioned to:

- Begin establishing a technical support organization for these software systems centered in the Washington, D.C., area.
- Expand the use of these visualization tools to build models of social networks that serve the needs of our diverse set of clients concerned with countering terrorism in all of its manifestations.

Non-Nuclear Energy Security

Through close coordination with IN, we will continue leadership of an early-stage multilaboratory program to address growing national concerns over non-nuclear energy issues affecting our secure energy future.
Specialized R&D

- **Development of Methods for Integration of Information, Imagery, and Multimedia Resources** - We develop and apply mathematical algorithms for automatic calibration and registration of geospatial intelligence information and massive data sets associated with information operations, exploitation, and warfare. Such methods are essential for automating registration of imagery from multiple sources and time periods to generate maps and imagery products for use by the intelligence analyst and the soldier.

- **Environmental Forensics Methods Development** - We will continue development of highly accurate laboratory methods for detecting and measuring radionuclides in the environment. Through application of statistical analysis, analytical radiochemistry, and related technologies, we enhance the nation’s ability to monitor and respond to nuclear events anywhere. This unique capability provides the U.S. government with an unparalleled radionuclide collection and analysis capability needed to monitor other nations’ compliance with nuclear explosion monitoring agreements.

- **Infrared Signatures Research** - Through internal investment, we are growing a new fundamental research capability to develop infrared spectral signatures for a wide variety of chemicals of concern to weapons proliferation, and for use in developing improved sensors and detectors for chemicals of concern.

- **Emerging Technical Challenges in Biometrics, Underground Facilities Detection and Characterization, and Small Power Source Needs** - A broadening cross section of our technical staff are providing innovative solutions to technical challenges related to small power sources for a wide variety of needs, advanced biometrics methods for security of assets, and development of new techniques for detecting and characterizing underground facilities.

- **Signatures in Coastal Regions** - Through a five-year congressionally directed funding supplement, we will expand our role as a developer of signatures intelligence capabilities in littoral or coastal regions at our Marine Sciences Laboratory in Sequim, Washington (Module 5.7).

Resource Requirements

Commensurate with proposed programmatic growth, we have begun internal planning to identify requirements and funding for enhanced secure laboratory facilities, communications, and computing resources to support an expanding classified program base in intelligence, defense, and homeland security mission areas between now and FY 2010.
4.5 Department of Homeland Security

PNL will be the government’s most effective national laboratory for bringing advanced S&T to bear on homeland security missions.

Harnessing the Laboratory’s Science Base

Achieving the needed levels of security to safeguard our homeland from terrorism without adverse impacts on the economy or individual rights poses enormous scientific and technical challenges. Our scientists and engineers are tackling the most daunting homeland security issues by using our capabilities in advanced chemical, nuclear, and biological detection; analysis and visualization of massive data streams; high-performance computing; and simulation and modeling of complex systems. Our portfolio of R&D initiatives also is providing significant, enabling contributions in many of these areas. We are providing the longer-term science and technology needed for continuous and evolving improvements to homeland security. The S&T are in the following four primary categories:

1. information analysis (early warning)
2. infrastructure protection
3. borders and transportation security
4. emergency management.

We will partner with end-users to apply our science base to counter threats and enhance mission operations. We will engage government, academia, and private sectors in the R&D needed for rapid prototyping and systems developments.

The Next Generation of Tools

DHS clients are turning to us to help create the next generation of tools that will be used by federal and regional agencies for early detection and prevention of terrorism. In response, we are focusing on analyzing complex streams of diverse information using our capabilities in information analysis and visualization with high-performance computing and advanced statistical methods. In the critical infrastructure arena—telecommunications, transportation, oil, gas, banking, and power grids—clients rely on us to ensure the continued operations of physical and cyber-based systems essential to the flow of commerce and government operations. As leaders in the cyber security field, our scientists are developing tools that focus on threat, vulnerability, risk, consequences, and recovery issues. Novel new tools also are being developed to provide simulation and modeling of complex critical infrastructures and their interdependencies.
Protecting our nation’s borders as well as air and seaports without impeding the flow of commerce is one of the most pressing issues facing the DHS. Our scientists and engineers are leading two efforts: 1) developing simple and robust, yet sensitive detections systems based on advanced nanomaterials technologies, and 2) leading the development, application, and integration of cost-effective solutions for efficient and effective detection of evolving threats to our borders, such as nuclear, chemical, or biological weapons or devices, or terrorists.

We also are teaming with DOE’s Hazardous Materials Management and Emergency Response facility to provide highly effective training for domestic and international border enforcement officials on methods to thwart the smuggling of materials around the world and in our homeland.

Resources

Exceptional programmatic growth in homeland security during the next five years requires critical infrastructure needs for secure computing and communication and a biosafety-level 3 (BSL3) laboratory capability. The application of secure computing to information sciences, modeling, and radionuclide data interpretation enables us to be a leader in each of these areas. State-of-the-art secure communications also allows us to maintain linkages with our various homeland security clients. To expand our leadership position in biosensors, we are proposing to operate a BSL3 laboratory, which permits breakthrough science with specific agents (see the proposed construction project table, Appendix B).

Scientists working in the Homeland Security Initiative at PNNL are developing highly selective adsorbent materials based on target analyte recognition to enable next-generation sampling, preconcentration, separation, and early detection capabilities for trace detection of chemical, biological, and nuclear threats.
4.5.1 Homeland Security Initiative

PNL’s novel “sensors-to-decisions” approach to detecting and preventing tactical and strategic terrorist threats and actions will result in the development of next-generation tools and methods to aid homeland security efforts.

S&T Roadmap

The Homeland Security Initiative is pursuing a multiyear roadmap of scientific and technological advancements leading to next-generation methods and tools for early detection and prevention of terrorism. The technical focus areas leading to these advancements are detection of chemical, biological, radiological, and nuclear materials and the dynamic analysis of massive, diverse information streams. In FY 2004 the scope of the Homeland Security Initiative will expand to include the development of bench-scale prototypes and initial software tools leading to a series of demonstrations. These demonstrations will bring together the results of all the initiative’s projects to address three scenarios: 1) attacks on the electric power infrastructure, 2) nuclear or biological contamination in drinking water and marine environments, and 3) early threat detection in a massive stream of intelligence information.

Sensing and Electronic Systems

The sensing and electronic systems aspect of the Homeland Security Initiative is focused on creating greatly improved detection and characterization systems for chemical, nuclear, biological, and radiological materials in geographically large and complex areas such as harbors, airports, sports arenas, and other buildings and structures. In collaboration with the Nanoscience and Technology Initiative and capability development efforts in nuclear S&T, techniques being investigated for material collection and preconcentration include supercritical fluid extraction, molecular imprinted polymers, and carbon nanotubes. Concepts being investigated for collection and sensing mechanisms include immobilized enzymes in porous nanostructures, sorbant nanosurfaces, single-chain antibodies, molecular-imprinted polymers, and single-enzyme nanoparticles. In FY 2004, these collection and capture mechanisms will be combined with optical and mechanical transduction mechanisms to create bench-scale sensing devices.

In parallel with these materials development and sensor creation projects, our staff are developing statistical analysis methods that integrate and exploit the data from multiple sensors. By exploiting differences in the collection and sensing mechanisms at the sensor-physics level and combining that information with information about how hazardous materials might be shipped or disguised, improvements can be made in both probability of detection and reduction of false alarm rates. Eventually, the resulting measurement capabilities will be combined with wireless communication electronics to create robust, field-ready measurement systems.

Predictive Analysis and Decision-Support Tools

The second focus area of the Homeland Security Initiative addresses capabilities needed to create a next-generation suite of predictive-analysis and decision-support tools for early detection of terrorist activities. Creation of these tools requires
pioneering advancements in methods for acquiring and analyzing dynamic information streams of unprecedented scale and complexity. These information streams may contain e-mails, documents, financial transactions, intelligence reports, images, and other information sources. Furthermore, the analysis process itself must change. Next-generation analysis must be done in new ways that engage human analysts and their computer-information-space tools in an interactive, dynamic dialog and investigative discovery process.

Research supporting these objectives is organized around four scientific themes: 1) automated data ingestion, 2) mathematical signatures and relationship discovery across diverse information types, 3) context and scenario analysis, and 4) visualization and human-information discourse. Portions of the research performed by the Computational Science and Engineering Initiative supports these objectives.

**Information Analysis Tools**

We are using this investment and a rich legacy of information science achievements to team with government agencies to develop a powerful, next-generation information analysis tool suite for use by federal, state, and local intelligence groups, and security and law enforcement agencies. To ensure that the tool suite can be easily adapted to a wide range of potential applications and end-users, a component software architecture is being used for all software tools. This approach ensures that the tool suite will be open, flexible, and easily adapted to the most complex or to more basic analysis requirements.

While the development of these next-generation information analysis tools and methods is an extraordinary challenge, creating a test bed where the performance of such tools can be evaluated poses an enormous scientific and technical challenge in its own right. As it becomes fully functional over the next one to two years, the Dynamic Information Analysis Laboratory (established in FY 2003 under this initiative) will provide a unique national resource for generating realistic threat information streams and evaluating threat detection algorithms.

In addition to their mission focus, the capabilities resulting from this initiative will have far-reaching impacts and benefits. The achievements in smart materials, sensors, and sensor-fusion methods are expected to benefit programs in environmental characterization, nuclear nonproliferation, intelligence, and process control. The investments in dynamic information analysis, visualization, and knowledge discovery will greatly strengthen our recognized national leadership in these areas and substantially increase our international recognition as well. In an information-rich, but often knowledge-starved age, the potential benefits and impacts of these advancements outside their original application domain are ubiquitous. Many diverse areas, including information-intensive scientific investigations, social sciences, human health and disease control, and commercial requirements could all benefit greatly from the advancements made by this initiative.
4.6 National Security Work for Others

PNNL will be a leader in development and application of fundamental sciences to detect, identify, interdict, and investigate chemical, biological, radiological, and nuclear threats smuggled across international borders, and to characterize, respond to, and recover from incidents involving weapons of mass destruction that occur outside the United States. We also will be the preferred source of criminal forensics and investigative support technologies for the U.S. law enforcement community.

Expanding Our Global Visibility

For the past several years, the U.S. Department of State has relied on us to:

- Develop and deploy advanced sensor technologies to detect weapons of mass destruction.
- Equip and train border enforcement officials from central and eastern Europe and the former Soviet Union to interdict and investigate those threats.
- Instruct first responders from five countries—The Philippines, India, Israel, Uzbekistan, and Kazakhstan—on the identification and mitigation of chemical, biological, and radiological threats.

We intend to increase the offerings from these successful programs, making the equipment and training accessible to a greater number of enforcement officials and first responders within more countries.

To accomplish these objectives, we will actively participate on international standards committees, at conferences and forums, and with intergovernmental organizations, such as the IAEA. We will offer enforcement officials and first responders the latest knowledge, more effective techniques, and innovative technologies. We also will use delivery and learning approaches that will increase student access to training, ensure consistency of training content, add value to the learning experience, and reduce the cost of training delivery. For example, a cognitive approach to "e-learning" will exploit computer-based and distance-learning technologies. Through interactive, experiential learning, a student's performance is improved by facilitating the acquisition and retention of knowledge, skills, and capabilities.

Forensic Tools

The successful investigation and prosecution of crimes require, in most cases, the collection, preservation, and forensic analysis of physical, trace, and digital evidence. We will continue to tap into our fundamental science base to provide the law enforcement community with unique or specialized scientific analytical capabilities and investigative support tools and techniques. For example, we are drawing on our core competencies in the chemical sciences and statistics to identify diesel fuel
fraudulently adulterated with nontaxable materials. The approach uses gas chromatography and pattern-matching algorithms to interpret assays of diesel samples. The results provide sufficient evidence for the U.S. Department of Treasury's Internal Revenue Service to thwart related criminal activities designed to avoid the payment of excise taxes. This work is being performed in partnership with the Laboratory for Chemometrics at the University of Washington.

We will continue to develop new scientific techniques, protocols, and equipment for performing analyses of forensic evidence with greater speed, sensitivity, and selectivity. We also will investigate ways to more clearly express statistics that often accompany evidence in trials. The statistical complexities are generally confusing and misunderstood by judges, jurors, and sometimes even by the experts themselves. Our intent is to enable federal, state, county, and city agencies with law enforcement responsibilities to perform their duties more effectively and efficiently, and to increase their solved crime and prosecution rates.

**Partnering for Success**

By applying the capabilities of multiple scientific disciplines and collaborating with scientists at other institutions, we will encourage our research staff to think creatively and pursue more innovative approaches. We also will establish industrial and market partnerships early in the development process to ensure that the resulting technology is rapidly prototyped, appropriately packaged and supported, and made commercially available to the law enforcement community in a timely and cost-effective manner.

The majority of our clients are federal government entities that are aligned with our market sectors. However, a number of unaligned government entities either directly or indirectly support national security functions and missions. They include various elements and agencies within the Departments of State, Justice, and Treasury.

Scientists at PNNL are using gas chromatography and pattern-matching algorithms to interpret assays of diesel fuel samples for the U.S. Department of Treasury’s Internal Revenue Service to detect evasion activities designed to illegally avoid the payment of excise taxes. The pattern-matching capabilities are being developed in partnership with the University of Washington.
4.6.1 Department of Defense WFO

PNL’s work for the broad spectrum of DoD clients enhances all of the Laboratory’s S&T capabilities for DOE missions.

From Science to Solutions

Basic and applied research programs for DoD science clients employ and improve our fundamental science capabilities in areas such as advanced materials and coatings, new sensor concepts, biological and chemical detection and characterization tools, and unique research in molecular processes. Our clients include the Defense Advanced Research Projects Agency (DARPA), as well as Air Force, Navy, and Army research laboratories.

Innovative Solutions for Energy

Within the energy arena, we provide DoD clients that have infrastructure and operating force needs with innovative technology solutions in power conversion, fuel cell and micro reactors, and heating and cooling technologies that range from the size of a pencil eraser to a breadbox. We also develop unique energy systems for buildings and vehicles, and power grid analysis resources. As a DOE lead laboratory for the Federal Energy Management Program, we provide analysis and services to DoD clients involving the use of advanced cost and energy conservation technologies in their infrastructures.

Solving Environmental Challenges

The pressing environmental challenges faced by DoD clients range from salmon-recovery issues and detecting and removing unexploded ordinance to characterization and remediation of sites. Our scientists and engineers perform applied environmental research under the Strategic Environmental Research and Development Program that creates new technology options for both DoD and DOE. We also define the science base for DoD clients who balance a diverse array of issues, such as environmental impacts, power generation, irrigation, military operations, and endangered species in regional watersheds and at defense sites.

There are many parallel programs between our robust national security work for DOE and for the armed forces. These areas include infrared sensors; nuclear, chemical, and biological detection and decontamination; cyber technology; information analysis systems; and meeting defense needs in homeland security and countering terrorism. Army, Navy, and Defense Threat Reduction Agency clients also draw upon our unique skills to solve problems in advanced materials, specialized sensor and electronics, radar imaging and smart radio frequency tags, logistics systems, and prognostic and diagnostics tools.
From basic research and energy to environment and national security, scientists and engineers are drawing upon capabilities in all of PNNL's mission areas to solve critical DoD issues.
4.7  Mission-Critical Infrastructure Resources

We must maintain and update our capabilities to address compelling national security challenges.

Maintaining Critical Capabilities and Facilities

To support defense nonproliferation mission objectives, we must provide critical radiological capabilities, establish classified intranet and Internet computing capabilities, invest in classified high-performance computing, and continue investments in core facility infrastructure at the Richland and Seattle, Washington, campuses.

High-Performance Computing

Efforts are under way to install and have operational by early FY 2004 a 64-gigaflop-cluster computer in the 3760 Building vault to support high-performance classified computing. This capability will allow processing of classified information at a high rate (24 hours a day, 7 days per week). To address projected growth at the Seattle campus, alternative office space leases are being considered. Several potential locations are under consideration that can enhance our proximity to strategically important private sector entities, provide long-term growth space, add improved facility infrastructure capabilities, and include appropriate space to allow establishment of limited area offices and computer laboratories to support classified program activities as business needs warrant.

Supporting Growth

PNNL needs additional office and computational space to support continued growth on the Richland campus. Specifically to meet continued demands for additional classified laboratory workspace, a $2 million capital project to renovate the 329 Building C-Section is proposed for FY 2004. This project would add more limited area laboratory and office space through renovation of currently underused/inefficiently used spaces in the facility to support continued growth and expansion of current programmatic activities related to our radiation detection and analysis and radiochemistry capabilities. PNNL also proposed renovation of a 331 Building laboratory to add BSL3 capability.

Investing in Classified Facilities

To support special programs mission objectives, we will make classified facility infrastructure investments at the Sequim, Seattle, and Richland, Washington, campuses to either establish or increase limited area, Secured Compartmental Information Facility (SCIF), and classified intranet and Internet computing capabilities. Efforts are under way to install classified networking capabilities through use of the DoD Secret Internet Protocol Router Network (SIPRNet).
at the Sequim and Richland facilities. Additional SIPRNet access terminals can be added at other facility locations on both campuses as programmatic needs warrant and funding becomes available. To increase classified processing capabilities at Sequim, conceptual design efforts are under way to convert a 1100-square-foot area in the Marine Sciences Laboratory 5 building to accommodate a small SCIF, additional limited area offices, and a classified conference room. These modifications would be funded by Battelle.

PNNL needs the resources and infrastructure to continue growing, evolving, and adapting to meet a variety of national homeland security mission needs. For example, at the Marine Sciences Laboratory (shown in picture) in Sequim, Washington, PNNL is increasing its classified processing capabilities by developing a conceptual design for converting an area of one of its buildings into a Secured Compartmental Information Facility, additional limited area offices, and a classified conference room.
5—Environment
5.0 PNNL’s Environmental Mission

PNNL provides solutions to DOE’s most critical national cleanup problems and will expand the application of our capabilities to address other national and international environmental challenges.

Several significant changes within DOE are affecting PNNL’s environmental mission area. First and foremost is the change of cleanup focus to risk reduction through cleanup and removal rather than risk management through physical and institutional controls. The implication of this change is that the DOE’s Office of Environmental Management (EM) is focusing on solving short-term problems and eliminating infrastructure with significant life-cycle surveillance and maintenance costs. A second significant change within DOE is the focus on establishing performance-based incentive-fee contracts with very aggressive performance targets for acceleration of cleanup baselines and the reduction of life-cycle costs. Lastly, there is a renewed emphasis on significantly increasing the participation of small businesses; many large contracts are being let as small-business set-asides. These changes signal a significant shift in environmentally related S&T investments—from longer-term S&T development to shorter-term S&T insertion.

As the only national laboratory employed by Hanford Site contractors to use S&T to impact technical solutions to cleanup challenges, our performance history shows that we are DOE’s leader at developing science-based solutions to critical environmental problems. As DOE’s leading environmental laboratory, we will continue to fully support DOE’s efforts to deal with its environmental legacies. In addition, we will draw upon our substantial multiprogram base to expand our support of key national and international environmental challenges that affect this country and the world.

Restore: Cleaning Up the Legacy of Nuclear Weapons Production

Our S&T contributions will substantially reduce the cost, time, and risk associated with restoring the environment by cleaning up the legacy of nuclear weapons production and enabling site closure decisions that have a sound, scientific basis.

We play a vital role in DOE’s efforts to protect the Columbia River and transition the Hanford Site’s Central Plateau into a modern waste management complex. Using our advanced environmental simulation capabilities to understand the groundwater systems, we have developed a system assessment capability that is rapidly becoming the risk decision tool at the Hanford Site. We are contributing to the development and demonstration of novel technologies for the retrieval, treatment, and disposal of high-level waste from underground storage tanks, as well as providing answers to key technical questions associated with the processing and disposition of spent nuclear fuels and sludge, and the closure of the contaminated fuel storage basins. Our S&T is instrumental in stabilizing the inventory of plutonium (Pu) and deactivating Pu facilities, as well as supporting the transuranic (TRU) waste retrieval and processing efforts at Hanford. Lastly, we are developing the new S&T necessary to address future environmental problems (Modules 5.1.1 through 5.1.5).
Protect: Protecting Workers, the Public, and the Environment

We will protect ecological and human health by ensuring the safety of the workers performing those cleanup activities as well as the protecting the public and the environment adjacent to cleanup sites.

Our efforts are contributing to the timely opening of a safe permanent storage facility for the nation's high-level nuclear wastes. We provide the scientific basis, along with credible data and models for monitoring and managing environmental and public risk resulting from residual contamination at DOE sites. Additionally, the leading-edge science, technology, and critical technical services that we provide to DOE helps ensure that cleanup is performed effectively while protecting the health and safety of the workers, public, and environment (Modules 5.2, 5.3, and 5.4). Our role in protecting workers, the public, and the environment goes beyond DOE cleanup challenges, however. For example, our work at the Marine Sciences Laboratory located in Sequim, Washington, is critical to developing U.S. Environmental Protection Agency (EPA) protocols to determine the effects of trace levels of contaminants on the endocrine and reproductive systems of organisms (Module 5.5).

Sustain: Renewing the Environment for Future Generations

Our S&T will help sustain the global environment by providing tools and technologies to address this nation's most challenging natural resource problems—ecosystem protection and management, carbon management, and water stewardship—in ways that are economic and enhance the quality of life.

We deliver basic and applied science to the EPA and the Army Corps of Engineers through R&D tools that allow jobs to be performed with greater confidence and effectiveness, and provide significant returns through technology transfer (Module 5.5). Our strategic alliance with the Mexican Petroleum Institute is working to deliver environmental S&T to the oil and gas industry, as well as developing joint research and development programs of mutual importance to the United States and Mexico that will address issues of ecosystem health in the Gulf of Mexico, the dynamics of climate change and the carbon cycle, and an understanding of methane hydrates for the future hydrogen economy (Module 5.5). We are developing technologies that use rapid heat and mass transfer at the microscale to improve performance, reduce cost, enhance safety and security, and minimize the environmental legacy for energy and chemical processes (Module 5.6). We are also developing innovative processes to convert biomass resources into higher-value chemical products and fuels, thus reducing the nation's requirements for petroleum and enabling the economic viability of DOE's biorefinery concept (Module 3.1.3).

PNNL is developing key technologies, such as those needed to retrieve and treat high-level tank waste, to protect the Columbia River and surrounding environment.
5.0.1 Environmental Mission Funding and Staff

While maintaining the capabilities to support DOE-EM's ongoing needs, we are redirecting some of our environmental capabilities from completed DOE-EM cleanup projects to address emerging national environmental challenges and homeland security needs.

As DOE moves to performance-based, incentive-fee contracts, the need for long-term R&D is expected to decline, while the need for short-term S&T insertions is expected to increase. This new approach is resulting in major changes in the funding and staffing profiles for our environmental work. Because of the high priority of the EM mission, we are committed to ensuring that we have the capabilities in place to provide ongoing support and to be able to respond to additional needs that may emerge in the future. We are transitioning our capabilities to address emerging national environmental needs as well as environmentally related needs in homeland security.

Environmental Quality

As the figure shows, we expect EM funding to decrease to $68 million in FY 2004 and to further decline over the next 5 years to $45 million in FY 2008. This reduction reflects contract completions and the shifting of work away from national laboratories to small and commercial contractors. We also expect the EM support to safeguards and security of $9.6 million to shift to the DOE Office of Science (SC) in FY 2005. However, we are currently projecting that some of this reduction will be offset by increased funding expected from the newly established, performance-based contractors at the Hanford Site and other DOE sites. We expect funding from these sources to increase from $4 million in FY 2004 to $17 million during the 5-year planning period. This work will include science and technology insertion for waste remediation at other DOE sites, and S&T roles on new maintenance and operation contracts for environmental remediation and restoration.

Other DOE Missions

We expect to maintain modest support to DOE's Office of Environment, Safety and Health (EH) over this period and to increase our support to the DOE Office of Civilian Radioactive Waste Management (RW) repository program to $3 million or more per year. This support will entail laboratory waste form testing, performance assessments to predict environmental impacts, transportation planning, and support to NRC licensing activities.

Environmental Research for Other Federal Agencies

We are projecting our environmental work for other federal agencies to increase to $5 million in FY 2004, and then increase further over the next 5 years to
$6 million. We expect this growth to occur with the EPA in the areas of computational toxicology and endocrine disruptors, multimedia/intermedia modeling, remediation technologies, water security and water resources, human-health and ecological risk, metals analysis, and homeland security and vulnerability assessments. Growth with the Corp of Engineers is expected in the area of sustainable management of ecologic systems, including endangered species. Also, over the planning period we expect our non-1830 work to increase from $17 million to more than $30 million.

**Staffing**

The additional programs for other federal agencies, as well as support for DHS and other associated homeland security agencies, will use many of the staff transitioning from completed EM research programs. Other staff from these completed programs are being used to support the growth envisioned in our energy programs, particularly in the areas of bio-based products and microtechnologies. We currently expect limited to no reductions of force over this time period due to the currently envisioned program changes.

Projected PNNL environmental mission funding and direct charged personnel through FY 2008. Near-term declines are projected as EM work declines and capabilities are redirected to non-EM work.
5.1 Technology Development and Deployment for DOE’s Environmental Management Mission

PNL leads the development of scientific and technical solutions to critical problem sets that advance effective cleanup at key DOE sites.

EM is accelerating its waste cleanup efforts by focusing on immediate results. EM contractors are developing risk-based, end-state cleanup and closure strategies that could result in higher levels of residual wastes at selected sites. Simultaneously, EM is reducing the role of centralized technical assistance and technology development projects in the cleanup program. Intractable problems remain, however, and the accelerated cleanup program will require future R&D investments specific to individual site needs.

Targeted R&D projects will be developed as needed by Hanford Site contractors using teams involving industry, national laboratories, and universities. These projects will include short-term technical assistance efforts to solve baseline technology problems and longer-term R&D efforts to make incremental improvements over existing baseline performance or to create breakthrough alternatives for intractable problems. In addition to solving specific problems, DOE site managers and their contractors need mechanisms to integrate R&D efforts and products across sites to leverage work done by others and to avoid redundant efforts to solve the same or similar problems.

We will use our relationships with other Hanford Site contractors to understand obstacles critical to EM mission completion. Where we believe our capability is the best to provide a solution, we will perform the work ourselves. Many problems, however, may require a select team of investigators from multiple organizations and disciplines. In these cases, we will use our established relationships through the ELC, consisting of representatives from 10 laboratories and two major cleanup contractors, to assemble a team of investigators appropriate to the problem. In addition, we will use our leadership position in the ELC to foster cross-site collaborations and information sharing to address integration issues to solve problems with the best available team.

With our experience in tackling complex cleanup problems and outstanding scientific staff and facilities, we will continue our leadership role as a key provider of EMSP-funded science (see Module 2.2.3). At Hanford, research supported through fundamental science programs such as EMSP is helping to develop key scientific insights such as a molecular-level understanding of the surface chemistry and reactivity of environmentally important mineral phases. This knowledge can be

(a) Intractable problems are 1) problems for which the knowledge/technology does not exist to address them, 2) problems that cannot be addressed within available time or budget constraints, and 3) problems that cannot be addressed without exposing workers/public to unacceptable risk or violating other regulatory requirements (Crowley, Kevin D. 2002. National Academy of Sciences, Science for EM Cleanup? Presented to the Office of Science Biological and Environmental Research Advisory Committee. December 4).
incorporated into advanced contaminant transport models and will be essential in developing new strategies for controlling or mitigating the effects of subsurface contaminants. In the past 2 years, nearly 50 EMSP project reports by PNNL and other investigators have been cited in Hanford Site regulatory documents.

Our collaborative relationships with site cleanup contractors at Hanford, and our relationships with other national laboratories and contractors through the ELC, will enable us to continue to integrate alternative technologies and innovative solutions into the physical cleanup progress across the DOE complex.

The following modules illustrate the contribution of PNNL’s S&T capabilities and collaborative approaches to provide solutions to key problem sets resulting in protection of the Columbia River and acceleration of cleanup activities at Hanford.

PNNL scientific research, such as understanding and modeling the movement of tritium in the groundwater, is addressing DOE’s critical legacy problems by developing the scientific basis for cleanup activities.
5.1.1 Protecting Hanford Site Groundwater and the Columbia River

PNNL’s S&T contributions provide the basis for optimizing Hanford Site cleanup efforts and our advanced environmental simulation capabilities will be used as the risk decision tool at Hanford.

Understanding Contaminant Transport

At most DOE Complex sites, the single most important environmental pathway for human and ecological exposure to existing and future residual levels of contamination is the soil-groundwater pathway. At the Hanford Site, human and ecological exposure may occur where contaminated groundwater discharges into the Columbia River. To aid cleanup efforts, DOE needs better knowledge of the biological, physical, and chemical conditions that explain and control the distribution of radiological and hazardous chemicals through this environmental pathway.

In addition to understanding the environmental pathways, DOE needs to be able to quantify and communicate the aggregate impacts of multiple waste sites on existing and future environmental and human health risks for diverse human and ecological populations. These risks need to be evaluated for multiple cleanup scenarios to optimize future risk reductions. Future remediation decisions at Hanford will rest upon the scientific understandings we develop that support an easy-to-communicate, credible, and acceptable risk statement of future conditions. To develop these scientific understandings, we will assemble an integrated multidisciplinary team—including geochemists, hydrologists, geologists, ecologists, risk and decision analysts, and mathematical and computational scientists—whose work will inform and influence environmental remediation and stewardship decisions.

We are developing the scientific understanding of physicochemical processes and geologic factors that control the fate and transport of radiological and hazardous chemicals through the soil-groundwater-river environmental pathway. Our program is an integrated approach involving both laboratory and field studies. Our scientific knowledge of contaminant transport supports recent cleanup decisions that avoid unnecessary cleanup, thus allowing cleanup dollars to be spent more effectively.

Estimating Risk

We are developing the conceptual and mathematical models describing the soil-groundwater-river pathway. Cleanup of the more than 700 waste sites at the Hanford Site will be addressed by a comprehensive new tool that will predict the movement and fate of contaminants through groundwater, the vadose zone (the soil above the groundwater) and the Columbia River. The System Assessment Capability (SAC) is an integrated system of computer models and databases that assesses the impact of contaminants on human health and the environment. Instead of showing each waste site in isolation—as has been done in the past—SAC shows each waste site in context of how they contribute to future impact, thus leading to more comprehensive solutions.
Two sets of computer models are at the heart of SAC. The first set—the environmental model—simulates how contaminants move through the environment. The second set estimates risk and impact from those contaminants based on a contaminant’s persistence in the environment, its mobility, chemical form and toxicity, and where it appears in the accessible environment.

Our field and laboratory projects use applied and basic science resources to generate data and information to further both the scientific understanding needed to support decisions and actions, and the data gaps identified in the models. We leverage EM funds with EMSP-funded projects to address these critical issues and work as an integrated team with site contractors to “piggy-back” our science on their characterization and cleanup efforts. As a result, our scientific products have direct application to Site contractor project objectives and provide the scientific basis for environmental remediation and remedy selection. Our science-based advanced risk simulation project will be a key element for helping regulators and the public to determine whether the cleanup program has achieved its intended risk levels.

Our preliminary risk simulation models are now providing useful, but not perfect, information. However, the scenarios developed and modeled to evaluate alternative cleanup strategies are already supporting project decisions on Site priorities and cleanup approaches. Future work will broaden and deepen our scientific understanding of contaminant behavior in the Hanford Site environment and will refine our ability to simulate and predict future contaminant migration and subsequent risk.

PNNL’s S&T is addressing key technical questions associated with the movement and cleanup of contaminated groundwater and the protection of the Columbia River.
5.1.2 Accelerating Hanford Site Waste Tank Cleanup

PNL technical solutions for treating and disposing tank waste help reduce costs, technical and programmatic risks, accelerate schedules, and provide defensible technical bases for cleanup decisions to ensure protection of the public and environment.

DOE’s Largest Environmental Challenge

The Hanford Site has the largest volume of high-level radioactive tank waste in the United States, with the highest life-cycle cost for cleanup of any other program area and site within EM. With 177 underground storage tanks containing 53 million gallons of waste and 200 million curies of radioactivity, the life-cycle cost for cleanup has been estimated at nearly $50 billion over 50 years. Technical, programmatic, and budget issues have slowed the pace of tank waste cleanup over the past two decades. DOE’s challenge is to significantly accelerate the pace of cleanup, thereby reducing the environmental risks and life-cycle costs. Accelerating tank cleanup activities while ensuring protection of the environment, workers, and the public will require a solid foundation of S&T. We are providing that foundation through key technical and programmatic assistance to DOE and the Hanford Site cleanup contractors in all major areas of tank waste cleanup, including waste tank safety and storage, waste retrieval, waste processing and immobilization, and tank closure.

Safely Storing Wastes While Accelerating Retrieval

DOE’s aging waste tanks necessitate accelerated retrieval to reduce risks of future tank leaks and enable early tank closure and processing to significantly reduce environmental risks and costs. However, severely limited tank space necessitates a careful balance between retrieval and continued storage. We are providing a fundamental understanding of tank waste chemistry and rheology coupled with engineering capabilities in fluid dynamics, computational methods, and monitoring technologies to reduce technical and environmental risk associated with the storage, retrieval, and transfer of tank wastes.

Bringing Waste Treatment Capabilities Online

 Paramount to completion of the tank waste cleanup mission at Hanford is the construction and start-up of the Waste Treatment Plant (WTP) to immobilize both high-level waste for disposal at a national repository and low-activity waste for disposal onsite (Module 5.1.3 provides additional information about spent nuclear fuel processing). In support of this effort, we will continue to provide critical engineering expertise in tank waste mixing, pretreatment, and vitrification along with a scientific foundation in chemistry, glass science, and materials in support of the WTP contractor. These capabilities support final processing system and flow sheet design, equipment selection, and operational planning to reduce technical risks.

(a) This work is funded by Bechtel through Battelle’s 1831 use permit, and is included here because of its essentiality to the Hanford Site cleanup effort.
In addition to the WTP, the DOE’s tank farm contractor is pursuing supplemental processing capabilities for low-activity, low-level, and mixed TRU wastes to obtain early disposition of selected tank wastes. This capability may also supplement the WTP and enable significantly accelerated low-activity waste treatment at reduced costs. Our scientists and engineers will continue to provide critical support in areas such as tank chemistry, safety, separations, immobilization, and long-term waste form performance and disposal to enable the selection of appropriate supplemental processing capabilities.

Closing Tanks and Disposing of Immobilized Wastes

Waste retrieval and processing enables closure of emptied waste tanks, final disposal of immobilized low-activity wastes, and significant risk reduction relative to continued storage of liquid high-level waste. Our capabilities in subsurface sciences, modeling, risk, and decision sciences are helping integrate tank closure and disposal risk and decision analysis with final waste disposition decisions across the entire Hanford Site cleanup mission. Our capabilities and tools will continue to provide a basis by which DOE and the Site cleanup contractors can identify and analyze the cumulative impact of waste disposition decisions relative to individual program and project decisions, such as a tank farm closure.

PNNL’s S&T is supporting resolution of key technical issues within the WTP flow sheet and process design. Progress toward bringing the WTP online is evidenced by construction progress from January 2002 (top) and April 2003 (bottom).
5.1.3 Spent Nuclear Fuel Processing and Disposition

PNNL’s S&T provide answers to key technical questions associated with the processing and disposition of spent nuclear fuels and sludge and the closure of the contaminated fuel storage basins.

The K Basins, located in the Hanford Site’s 100 K Area, were used from the mid-1950s to the early 1970s for underwater storage of spent nuclear fuel generated by the site’s K Reactors. In 1975, the basins began receiving spent fuel from N Reactor. Associated with the storage of 2100 metric tons of N Reactor fuel, particulate material—referred to as sludge—accumulated on the basin floor, in fuel canisters, and in the basin pits. The approximately 52 cubic meters of sludge (the majority of which resides in the K East Basin) is composed of a mixture of fuel corrosion products such as metallic uranium and fission and activation products, small fuel fragments, iron and aluminum oxides, concrete grit, sand, dirt, and operational and biological debris.

Our researchers are assisting Fluor Hanford’s Spent Nuclear Fuel Program with the significant technical challenge of providing the underpinning science and data to establish defensible design and safety basis parameters for the retrieval, containerization, transportation, and storage of the sludge generated from metallic uranium-based spent nuclear fuel. As part of this support, we are performing laboratory- and bench-scale testing and conducting key studies and engineering evaluations, including determination of the uranium metal distribution and content in the various sludge types, determination of sludge thermal conductivity and shear strength, evaluation of corrosion-based volumetric expansion and gas retention during sludge storage, and formation and mitigation of vessel-spanning bubbles during sludge storage. Such studies will provide information needed to determine container fill levels, and to model and predict flammable gas generation and thermal stability of the sludge during containerization, transportation, and storage.

In tandem with the sludge characterization studies, our researchers are developing one-of-a-kind technologies for performing nondestructive evaluation of the highly contaminated fuel storage basins. Because radionuclides such as cesium can migrate deeply into the concrete walls, technologies are needed to determine the depth and extent of contamination before the basins can be decontaminated and decommissioned. A characterization system developed by PNNL has provided Fluor Hanford personnel with measurements of contamination from the floor area and the basin wall. These readings show significantly more contamination than originally estimated. Using our characterization data, Fluor Hanford is now proceeding with preparing its deactivation strategy.

As the K Basins approach sludge removal and deactivation, Fluor Hanford must develop documentation to define the project endpoint. The characterization data we provided is just one example of how the Laboratory is contributing to this endpoint decision process. Our risk and decision science capabilities will be instrumental during Fluor Hanford’s consideration of all endpoint decision criteria, including regulatory approaches, cost effectiveness for remaining work, and worker
and public safety. This information will provide the technical basis for making distinctions between processing and disposition options, balancing risks against cost and schedule, and developing a sound framework for making programmatic decisions.

Our support to spent nuclear fuel processing and disposal activities at Hanford will come to completion in FY 2004. Existing and future national and international spent nuclear fuel packaging, transportation, and disposition challenges will benefit from our expertise and understanding of the chemistry and physics of spent nuclear fuels and sludge.

PNNL is conducting laboratory- and bench-scale studies that help establish defensible design and safety basis parameters for the processing and dry storage of spent nuclear fuel sludge, and developing one-of-a-kind technologies to perform nondestructive evaluation of highly contaminated fuel storage basins in support of basin closure activities.
5.1.4 Plutonium Stabilization and Facility Deactivation

Stabilizing and disposition of plutonium and deactivating and closing contaminated facilities will continue to depend, in part, on PNNL S&T.

The Plutonium Picture

The Plutonium Finishing Plant (PFP) at Hanford once contained over 4 metric tons of plutonium in 17.8 metric tons of bulk plutonium-bearing materials left from defense production. The material is in a variety of forms including metals, oxides, liquids, and polycubes (plutonium bound in plastic). Under the oversight of DOE and the Defense Nuclear Facilities Safety Board, Fluor Hanford has made significant progress in stabilizing these challenging waste streams. During the past five years, our researchers have provided testing and laboratory support necessary to further understand the behavior of these materials and have developed or optimized several stabilization processes. While most of the stabilization effort has been completed, some of the most technically challenging waste streams remain.

In addition, approximately 1.1 metric tons of scrap plutonium oxide—generated by pyrochemical operations at the Rocky Flats Environmental Technology Site—are stored at the PFP. Here, they await thermal stabilization in PFP's furnaces before packaging and eventual offsite shipment and disposal. A significant portion of this scrap plutonium is composed of high-chloride oxide material, which—according to DOE-STD-3013-2000, Stabilization, Packaging, and Storage of Plutonium-bearing Materials—must undergo moisture measurement to less than 0.5 weight percent (to mitigate overpressurization within storage containers) and stabilization at a temperature of 950°C for 2 hours. However, at this higher temperature, chloride salt vapors cause severe corrosion to furnace heating elements and ventilation components, and plugging in the furnace's off-gas lines.

Stabilization Progress

To address the challenges associated with the highly corrosive plutonium oxides, our researchers are conducting laboratory studies to evaluate whether the plutonium oxides can be stabilized at lower temperatures, thereby minimizing volatilization of the chlorides while still meeting moisture-content goals of the prescribed national standard. If determined feasible, this stabilization method will eliminate the need to wash chloride-laden plutonium prior to processing, resulting in significant cost savings and reduced risk to Hanford Site workers, the public, and the environment.
In addition to providing laboratory and research support to the plutonium stabilization efforts, we will provide technical expertise in support of facility deactivation efforts at the PFP. Because the plutonium contained in this facility is not easily retrievable, future deactivation work is expected to involve significant radiological and industrial risks to the workers. To mitigate exposure risks, our researchers will evaluate unique robotics and remote cutting techniques, and dust suppression and fixative technologies. Additionally, we are leading efforts to evaluate technologies related to plutonium characterization and decontamination, especially technologies that are chemically based.

Much of our deactivation and facility closure support, including plutonium-removal processes, is expected to continue through FY 2006. It is expected that PNNL’s analytical and processing capabilities, developed in support of the Hanford mission, will be drawn upon as DOE continues efforts to disposition plutonium at the Savannah River Site. In addition, we believe there is direct applicability of our capabilities to other national and international nuclear fuel cycle challenges.

PNNL is working with Fluor Hanford to develop and optimize processes needed to stabilize some of DOE’s most challenging plutonium legacy materials, including the corrosivity of high-chloride plutonium oxides.
5.1.5 Retrieval and Processing of TRU Wastes

PNL’s scientific and technical capabilities are integral to developing impactful solutions to challenges faced by the TRU waste program at Hanford.

The Hanford Site has the second largest inventory of TRU waste in the DOE complex. Past projections state that cleanup of this waste could cost up to $1.7 billion and take more than 35 years to retrieve, treat, and dispose of the more than 13,000 cubic meters of remote-handled and oversized TRU waste, along with remote-handled mixed low-level waste at the Site. DOE is making a concerted effort to accelerate cleanup and reduce overall costs, and the Washington State Department of Ecology is keenly interested in DOE efforts to address the TRU waste cleanup.

The current site cleanup contractor, Fluor Hanford, has responsibility for the Hanford Site’s TRU waste programs, including characterization, retrieval, segregation, treatment, storage, transport, and disposal. The contractor’s current emphasis however, is on contact-handled TRU, with most of the high-risk remote-handled work scheduled to occur in the out-years beyond DOE’s current contract with Fluor Hanford.

The Hanford Site remote-handled TRU challenges include burial grounds that were operated for disposal of pre-1970 TRU and low- to high-level activity waste. Documentation of materials placed in the burial grounds is incomplete, but it is recognized that high-activity fission product, low-level, and mixed low-level radioactive waste, plutonium, uranium, and other TRU wastes exist in various waste forms. Capabilities for locating the boundaries of burial ground trenches are needed. Additionally, waste characterization and segregation technologies are needed to reduce cost and minimize worker exposure to radiation. We have the capability to provide key remote-handling and processing capabilities for this problem when DOE begins to address the TRU challenges. We are engaged in workshops to identify technical options and are viewed as a valued contributor to these solutions.

Through application of the SAC model (described in Module 5.1.1), our researchers are working with Fluor Hanford to identify the environmental and human health risks associated with TRU waste. The SAC technology shows each of Hanford’s waste sites in the context of how they contribute to future impact. This work will provide critical information necessary to reduce the risk to Site workers, the public, and the environment.

Our current and future focus is to apply our core technical competencies to address DOE and Site contractor challenges associated with risk identification and mitigation. Through the application of our core competencies in sensor/characterization development and application, robotics applications, radiochemical processing, and waste form development, we will drive S&T to application in support of the TRU waste retrieval and processing efforts at Hanford.
PNNL is providing environmental risk and decision science capabilities and technologies to address the significant worker health and safety risks associated with the storage and retrieval of high-level TRU. This figure provides examples of remote-handled and large-packaged TRU waste containers.
5.2 Disposal and Safe Storage of High-Level Wastes at Yucca Mountain

S&T contributions from PNNL help to ensure timely opening of a safe permanent storage facility for the nation’s high-level nuclear wastes.

The timely opening of a permanent waste repository that will accept high-level nuclear waste from EM cleanup programs is vital to the completion of the legacy cleanup mission. It is also vital to the continuation of the nation’s nuclear electric power generation because some of the nation’s commercial nuclear power and defense wastes require isolation from the environment for 10,000 years or more. Temporary storage of these materials at many current surface sites is costly and does not provide the long-term isolation necessary to reduce the risk of exposure to the public and the environment.

The Office of Civilian Radioactive Waste Management is currently focusing its efforts on the preparation of the NRC license necessary to operate the Yucca Mountain Repository, with submission of the license application planned for December 2004. Repository operations and the acceptance of the first high-level wastes are planned to begin in 2010. Our work in waste form performance provides strong support to this program objective.

Waste Form Performance Testing

Our outstanding scientific and engineering expertise in high-level nuclear waste spans the commercial nuclear power industry, reactor R&D, and nuclear defense activities. Key aspects of this expertise include an understanding of the long-term behavior of spent fuel and nuclear waste forms, the long-term behavior of radioactive materials in the environment, and the long-term impacts of radioactive contaminants on human and ecological health. In addition, an understanding of the development of innovative materials for the long-term containment of radionuclides; the insertion of technologies for the improvement of repository cost and schedule; and the development of safe, secure, and efficient transportation systems are also critical to solving high-level nuclear waste issues.

We have conducted waste form testing of commercial spent nuclear fuel and high-level nuclear waste for 17 years in the Radiochemical Processing Laboratory (RPL). Data generated in the RPL are being used to develop the performance assessment models that will be used to define how these waste forms will perform over the expected life of the repository. These models will also be used to evaluate the long-term safety of the repository itself.

PNNL Awarded Pilot Study from RW Science Program

The Office of Civilian Radioactive Waste Management has established an RW Science Program to broaden and deepen the repository scientific base. It is expected that this program will strengthen the safety and cost performance of the repository by allowing insertion of new scientific information during licensing, and new technologies during site construction and operations. As the recipient of a pilot study in the initial round of awards in the RW Science Program, our study focuses on the development of nanoporous “getters” for radionuclide containment. Getter materials have the potential to provide a cost-effective safety margin in addition to the waste package and natural barrier systems.
The application of PNNL’s S&T to the disposal and storage challenges posed by the Yucca Mountain site will help the site to become the nation’s repository for the permanent safe storage of high-level nuclear wastes from electric power generation and nuclear defense cleanup activities.

PNNL’s expertise in long-term behavior of spent fuel and nuclear waste forms, the long-term behavior of radioactive materials in the environment, and the long-term impacts of radioactive contaminants on human and ecological health will help DOE address problems associated with the transportation and long-term storage of high-level nuclear wastes at the Yucca Mountain High-Level RW Repository.
5.3 Monitoring Environmental and Public Health Risks

PNNL provides the scientific basis and credible data and models for monitoring and managing environmental and public risk resulting from residual contamination at DOE sites.

PNNL Monitoring Programs form the Scientific Basis for Demonstrating Public and Environmental Safety

DOE national laboratories and small and large cleanup sites are the stewards for significant pieces of real estate across the United States. These land holdings include sensitive ecological areas, are often located near major metropolitan areas, and are often perceived by surrounding communities as major sources of environmental contamination posing offsite human health and ecological risks. The need for science-based environmental characterization and monitoring efforts will continue indefinitely at sites with continuing missions, as well as at sites with residual contamination that are remediated to some risk-based end-state condition and released for alternative post-cleanup use. These characterization and monitoring programs form the scientific basis for communication programs seeking to credibly demonstrate public and environmental safety.

Ongoing monitoring programs supported by an adequate scientific understanding of environmental processes, risk assessment simulation, and prediction capabilities (see Module 5.1.1) form the scientific basis for determining risk-based end-states that describe the achievable endpoint of EM's cleanup programs. That is, the data and information generated by these programs and capabilities form the credible scientific base for evaluating acceptable residual contamination levels for optimal future alternative land use.

Site Monitoring Programs Provide Data to Enhance Development of New Monitoring Technologies

Our near-term stewardship monitoring programs at the Hanford Site are integrated with our ongoing field and laboratory environmental R&D projects that develop and model the scientific information on the future public health and environmental risk of post-cleanup residual contamination. These programs encompass the detection of radiological and hazardous chemicals related to site operations in soil, biota, surface and groundwater, air, and foodstuffs from the regional environment. In addition, our programs also monitor natural and cultural resources. The monitoring programs provide characterization information to the R&D projects and in turn use the scientific and technological outcomes of the R&D to refine monitoring approaches. The outcome is an optimally scoped credible monitoring program that increases public assurance of human health and environmental safety.
Future R&D, focused on monitoring program-derived needs, will lead to more effective, cost-efficient, long-term monitoring programs by developing new monitoring technologies and protocols and an improved scientific basis for what to monitor, how to monitor, and where to monitor. One innovative example currently under development is the environmental sentinel initiative. Essentially highly sensitive, highly contaminant-selective detectors, environmental sentinels will detect and identify biological community responses to contaminants at levels below those deemed harmful, thus providing an early warning mechanism to trigger remedial intervention.

To meet our customers’ future needs, including the need to accelerate the Hanford Site cleanup schedule, we will develop monitoring capabilities required for cost-effective stewardship of residual wastes present at DOE sites, targeting ecological resources rather than the chemical inventory itself.

PNNL provides scientific leadership for developing effective, cost-efficient site monitoring programs. Our Hanford Site monitoring programs encompass the detection of radiological and hazardous chemicals related to site operations in soil, biota, surface and groundwater, air, foodstuffs from the regional environment, and natural and cultural resources.
5.4 PNNL’s Role in the Health and Safety of Hanford Site Workers, the Public, and the Environment

Through its technical services and applied research, PNNL creates technologies and solutions leading to a healthier workforce and more sustainable environment.

We provide S&T and critical technical services to DOE to ensure that Hanford Site cleanup is performed effectively while protecting the health and safety of the workers, public, and environment. We leverage our fundamental research in biosciences to address worker monitoring and to predict possible health effects from environmental exposures. Our support is critical because it is based on federal requirements, meets DOE liability issues, addresses concerns raised by workers, and ultimately reduces cleanup life-cycle costs.

Personnel Monitoring

We provide the personnel radiation dosimetry services for the entire workforce on the Hanford Site. These services, which meet the federal requirements as stated in 10 CFR 835 and certified by the DOE Laboratory Accreditation Program, have allowed us to develop a deep understanding of technical issues surrounding personnel monitoring. This understanding has led to S&T programs that have resulted in fundamental advances in health physics and radiation dosimetry. For example, we recently created an entirely new approach to radiation dosimetry using Optically Stimulated Luminescence. This new technology was successfully transferred to industry.

The next Grand Challenge in personnel monitoring is in the area of chemical dosimetry. As cleanup begins in earnest within the DOE complex, an area of great concern is chemical exposures to the workers. With thousands of chemicals in the DOE complex, determining individual exposures to a wide variety of chemicals is extremely difficult. We are meeting this challenge by integrating expertise in personnel dosimetry, chemical toxicology, biomarker research, and microtechnology to develop real-time, noninvasive personnel monitors for chemical exposures. We are partnering with the cleanup contractors and the onsite medical provider, Hanford Environmental Health Foundation, to develop and demonstrate new technologies that can eventually be used as part of the worker medical surveillance program.

We calibrate and test portable radiation survey instruments for the Hanford Site. These onsite services have enabled the Site contractor to have immediate access to qualified equipment in a cost-effective manner. The calibrations are performed in a National Institute of Standards and Testing-certified calibration facility in the 300 Area, the only such certified facility in the DOE complex. The specialized testing that occurs in this facility has led to enhancements on current instruments and novel developments for new instruments. Most of the testing has been with ionizing radiation instrumentation, but some industrial hygiene instrumentation has also been tested. As chemical monitors are developed, this facility will be used to test and enhance those as well.
Radiation Records and Dose Reconstruction

We maintain personnel radiation dosimetry records for all past and present workers on the Hanford Site. More than 100,000 records are kept on file in an easily retrievable system that has been instrumental in Hanford’s ability to successfully respond to the National Institute for Occupational Safety and Health’s request to the DOE for radiation exposure records as part of the Energy Employees Occupational Illness Compensation Program Act. We provide the necessary health physics expertise to interpret and analyze these records for the client.

We are recognized internationally in radiation dose reconstruction. We are supporting the EH by performing dose reconstruction for workers and the public near Mayak’s processing facility in the former Soviet Union.

Health Risk Assessment: By integrating our expertise in fate/transport modeling, exposure characterization, dose assessment, and health effects studies, we are able to better determine the overall health risk attributed to an individual due to multiple exposures. For instance, we are conducting chemical toxicology assessments of vapors in the Hanford Site tank farms and their potential effects on workers and the public. In the future, we plan to build upon our knowledge in the biological sciences to study the effects of these chemicals on individual cells, extrapolate that data to whole organs, and eventually determine health outcomes to individuals and sets of subpopulations. This research will lead to better decisions regarding cleanup levels and exposure standards.

The Hanford Site contains 177 underground radioactive waste tanks, the contents of which are routinely monitored by highly trained workers. PNNL provides radiation measurement tools to protect Hanford Site workers by monitoring their exposure to radiation.
5.5 PNNL's Environmental R&D WFO

PNNL delivers additional value to DOE by conducting environmentally related research and development for other government agencies and private clients.

Environmental Protection Agency

We conduct a variety of research to assist the EPA in its central role of developing, implementing, and enforcing environmental regulations. This research includes modeling and analyzing hazardous waste transport and fate in soil, water (both fresh and marine), air, and biota; developing human health risk assessment information, methods, and guidance, as well as improving the science and practice of risk assessment; and developing innovative compliance information tools for government and industry.

Our work for the EPA is directly related to, and complements, our environmental science research for DOE. This work includes assessing the technologies and economic impacts of selected international strategies to reduce greenhouse gas emissions; developing innovative pollution prevention design, management tools, and methods; integrating disparate databases, and models, multiple-media models, and software-assessment frameworks; assessing the impacts of global climate change; and developing and supporting new and innovative techniques for metals analyses and bioassays.

We intend to be involved with the newly formed EPA National Homeland Security Research Center, whose mission focuses on methods to clean up contaminated buildings, protect the nation’s drinking water supplies, and improve risk assessment methods that protect emergency responders and inform local decision-makers. The new center works with other federal agencies, the academic community, and the private sector to incorporate all available technical expertise and technological advancements into its research programs. We anticipate coordinating the efforts of EPA’s Environmental Technology Verification program with those activities associated with the PNNL’s Homeland Security Initiative.

Army Corps of Engineers

During the last 20 years, we have performed in-depth research and technology development to help resolve critical decisions affecting water resource management, especially hydroelectric dam operations in the Pacific Northwest. These decisions, which often involve the conflicting needs of industrial and agricultural development versus the safeguarding of fish and wildlife species, continue to be major issues faced by the Army Corps of Engineers and DOE. Our work for the Corps of Engineers (primarily in the Portland, Oregon, and Walla Walla, Washington, Districts) provides the scientific basis for many key decisions faced by managers and operators at hydroelectric dams located in the Columbia and Snake River Basins. The key issue at these dams is the safe passage of juvenile salmon moving downstream.
The Corps of Engineers work is the major component of a larger regional water management program that also includes work for DOE’s BPA and Wind/Hydro Power program, as well as regional private utilities. The Corps of Engineers provides substantial programmatic support to develop facilities and equipment that directly benefit these DOE programs.

**Oil and Gas Industry**

The international oil and gas industry as a whole faces significant environmental and safety issues. Included in this list are the need for environmental assessments, pipeline integrity and management (natural gas and oil pipelines), pipeline transmission, refinery operations, well logging and drilling, extraction, exploration, sustainability, production, health and safety, and emergency planning and operation systems. These issues are critical to understanding ecosystem health in key areas such as the Beaufort Sea (Alaska) and the Gulf of Mexico, among many others. Oil and gas exploration and production practices will have a direct impact on climate change and the carbon cycle. In addition, as the United States moves toward the future hydrogen economy, DOE, other resource agencies, and multinational oil companies will be interested in the potential role of methane hydrates in the carbon cycle and as an energy source.

Many of the tools and techniques we have developed and applied to environmental challenges at the Hanford Site (and the larger weapons complex) and elsewhere in the Pacific Northwest apply directly to the needs of the oil and gas industry. These capabilities include environmental chemistry, remote sensing, bioassays of sediment and water, fisheries monitoring and population modeling, and socioeconomic development analyses.

In collaboration with the Mexican Petroleum Institute, we will identify joint research activities to address key issues associated with the long-term cumulative impact of exploration on the Gulf of Mexico ecosystem, the dynamics of climate change and the carbon cycle (a deep drilling hazard) in the Gulf. The results of this work could be of significant benefit to SC, the DOE Office of Fossil Energy, EPA, the National Oceanic and Atmospheric Administration, and the Minerals Management Service, the latter which is responsible for the U.S. outer continental shelf oil- and gas-leasing program.

PNNL developed sensor-packed synthetic salmon that are making their way through the turbines at Bonneville Dam and other hydroelectric projects to measure the conditions that real fish encounter as they pass through turbines at hydroelectric dams on their way to the ocean. The information they collect could lead to more fish-friendly turbines in the future. Photo credit: Bonneville Dam and salmon smolts are courtesy of the U.S. Army Corps of Engineers.
5.6 Microscale Phenomena for Sustainable Environmental Quality, Energy Delivery, and National Security

Through technologies that use rapid heat and mass transfer at the microscale, PNNL is improving performance, reducing cost, and enhancing safety and security for energy and chemical processes.

Using Microscale Phenomena

More than a decade ago, our researchers began exploring the potential advantages of engineering systems to take advantage of the rapid heat and mass transfer that can occur over short length scales (nominally, 5 to 100 microns). The advantages of process engineering using microscale phenomena are now being realized over a wide range of applications, for DOE as well as other federal agencies and commercial groups. However, the challenges associated with widespread development and use of microscale phenomena require the development of a body of scientific and technical knowledge, and skilled practitioners of that knowledge. We will continue to explore and develop the body of knowledge associated with microscale phenomena and apply that knowledge to major challenges facing the nation.

Microproducts Breakthrough Institute

We teamed with Oregon State University (OSU) to form the Microproducts Breakthrough Institute. This Institute will advance scientific and technical knowledge in microtechnology, and when possible, the transfer of related technology to Northwest industry. With OSU, we will use our respective facilities, education, and training programs to conduct research and form multidisciplinary teams. The Institute will facilitate more rapid exploration of the science and engineering of microscale phenomena, and technology development and commercial deployment to meet national needs. It will also enhance the translation of scientific and engineering discovery related to microscale phenomena into a body of knowledge and focused educational curricula to rapidly disseminate that knowledge.

Examples of the application of microscale process engineering follow.

Fueling Hydrogen Transportation

We are developing fuel processors and reformers for use in automobiles. These reformers take advantage of the rapid transport achievable at microscales to achieve more selective and energy-efficient conversion of hydrocarbon fuels to hydrogen and carbon dioxide. The dramatic reductions in size (factors of 10 to 100) are particularly important for transportation applications. Additionally, the development of heat exchangers employing microscale heat transfer phenomena allows
extremely high process intensification (heat transfer density exceeds that associated with a commercial nuclear reactor) and associated miniaturization. Work is under way to complete component development and then achieve integrated designs that will further improve performance.

While particularly well suited for onboard reforming of hydrocarbon fuels, the technologies provide advantages associated with process efficiency, footprint, safety, and cost for stationary fuel processing as well.

**Small power**

High process intensification, integration, and miniaturization have substantial potential to dramatically enhance development of small power systems. We have developed systems ranging from 30 megawatts to 200 watts for applications in sensor and man-portable power, primarily to replace battery power. These developments have principally been in support of the Defense Advanced Research Projects Agency and Army/Marine Corps programs. In general, miniature fuel reformers have been developed to provide hydrogen for fuel cells. The integrated systems have been projected to have over five times the power density of advanced batteries for missions of interest to the military.

**Absorption Heating and Cooling**

We are using integrated microscale chemical and thermal processes to develop absorption cooling technology for man-portable cooling. Such technology would dramatically ease the challenges of conducting either armed conflict or emergency response in hazardous environments, particularly for chemical and biological hazards. Through funding from the Army, we are teaming with OSU to use distinctive capabilities in the development of man-portable cooling systems. The development of such systems requires microprocess engineering skills and use of advanced simulation tools employing lattice-Boltzman techniques for simulation of absorption and desorption phenomena at microscales. This technology also holds great potential for improving efficiencies in thermally activated cooling systems for automotive, residential, and commercial building heating and cooling units.

**Enhancing Space Exploration**

We are developing several technologies for NASA that will dramatically enhance manned and unmanned exploration of space. Technologies that will improve fuel cell performance, provide for liquid vapor separations in zero-g, and do chemical production of propellants from indigenous materials on Mars are the topics of current research. The development of these technologies will have significant terrestrial applications, augmenting development described earlier for application in transportation, stationary energy, and national security missions.
5.7 Extending PNNL’s Environmental Reach

PNNL is expanding its environmental reach into new areas including the development of biobased products and processes that will develop innovative processes to convert biomass resources into higher-value chemical products and fuels, coastal security, and key environmentally related transportation issues.

Bio-Based Products and Processes

Through our Bio-Based Products and Processes program, we develop innovative processes to convert biomass resources into higher-value chemical products and fuels, thus reducing the nation’s requirements for petroleum and enabling the economic viability of DOE’s biorefinery concept. We draw upon our distinctive chemical and biological catalysis capabilities to support R&D of processes that would allow readily available biomass resources to displace petroleum as a feedstock for chemicals and ensure the financial viability of ethanol production in large, integrated biorefineries.

We are the lead DOE laboratory for developing chemical intermediates and other industrial products in conjunction with industry partners via cost-shared Cooperative Research and Development Agreement projects that focus on rapid technology proofs-of-concept and demonstration of commercial viability. Building upon fundamental knowledge of catalytic processes and formulation, including advanced biocatalysis techniques, we will capitalize upon both SC and the DOE Office of Energy Efficiency and Renewable Energy (EERE) assets to develop the next generation of conversion processes, leading to new families of industrial and consumer products, reducing the nation’s dependence on imported petroleum, and helping create a new bioindustry. We will continue to develop and demonstrate innovative, breakthrough catalyst formulations and catalytic systems and we will provide leadership in assisting DOE in setting programmatic direction focused on the next generation of biofuel and bioproducts technologies. More information about our Bio-Based Products and Processes program can be found in Module 3.1.3.

Sequim Growth Agenda and Coastal Security

Our Marine Sciences Laboratory, located in Sequim, Washington, provides a nationally recognized analytical capability in the fields of marine chemistry, ecotoxicology, and coastal restoration. Because current facilities at the Marine Sciences Laboratory are limited, a new multi-use laboratory and office facility are proposed that can accommodate new business. The new facility will capitalize on the outstanding environmental assets of this location. The new laboratory will use “sustainable technology” to minimize waste production and emphasize the use of such things as ambient light, solar heating, recycling/reuse and other “green technologies.” This state-of-the-art research laboratory will meet DOE and DHS needs for the next 10 years.
Washington State Department of Transportation

Our activities in the growing transportation sector serve to meet the needs of America’s transportation systems. Our major focus is helping Washington State solve major environmental and natural resource problems for local highway systems and the Puget Sound. Our relationship with the Washington State Department of Transportation (WSDOT) leverages our work with other key Northwest clients, such as the Army Corps of Engineers and BPA, to help resolve some of the region’s most difficult energy, transportation, water resource, and ecological issues.

A key example of this work is finding a more fish-friendly design for future stream crossings and for the thousands of culvert retrofits expected to be completed in coming years. The WSDOT, representing a consortium of West Coast transportation agencies, has contracted with us to design and install a culvert test bed in south-western Washington. The full-scale, one-of-a-kind culvert test bed system allows scientists to adjust and measure the hydraulic conditions—water velocity, turbulence, and depth—of various culvert designs. By assessing different slopes and flow regimes, scientists can determine how these conditions influence fish behavior and the ability of the fish to pass through a variety of culvert designs being considered as retrofits.

On a larger front, our U.S. Department of Transportation (DOT) business also provides solutions to some of the nation’s major transportation problems involving safety, efficiency, and environmental acceptability. Key clients include the DOT, its several agencies, other federal and state transportation agencies, and the commercial air-land-sea transportation industry.

Visitors inspect the full-scale, one-of-a-kind culvert test bed system located at the Washington Department of Fish and Wildlife Skookumchuck Hatchery near Tenino, Washington. Impacts to juvenile salmon during passage through culverts represent a significant Endangered Species Act (ESA) issue for Pacific states. The test bed enables controlled experiments that will yield the behavioral and hydraulics data to address this ESA issue.
5.8 Infrastructure Needed to Support the Environmental Quality Mission

Targeted facility investments will enable PNNL to continue to provide expertise in radioanalytical processes and ecological research, and to support bioproducts science and engineering efforts.

Infrastructure Needs

To maintain capabilities critical for supporting DOE’s environmental quality mission, targeted facility investments are needed. We currently have key facility needs in three areas: radiological and environmental laboratories; the Marine Sciences Laboratory in Sequim, Washington; and the proposed Bioproducts, Sciences, and Engineering Laboratory (BSEL).

Radiological and Environmental Laboratories

Underground tanks at the Hanford Site contain some of the most highly concentrated radiological waste in the nation. To ensure future environmental and public health protection, these materials must be isolated from the environment for thousands of years. To immobilize contaminated tank contents into a glass matrix, the design and construction of EM’s WTP relies heavily on work performed in the RPL.

Contaminants already released to the soil and groundwater at Hanford represent the most likely potential environmental and public health risk. Understanding the fate and transport of these contaminants through the soil-groundwater pathway is key to helping complete EM’s mission to remediate the groundwater and protect the Columbia River for future generations. Environmental laboratories in the RPL provide the sophisticated radioanalytical capabilities necessary to understand the subsurface biogeochemistry that controls the fate and transport of radionuclides in the soil.

To ensure the availability of this important capability as the 300 Area transition takes place, we plan to add new facilities with state-of-the-art radiochemical and analysis laboratories. See Module 7.3.2 for more information.

Marine Sciences Laboratory

Our Marine Sciences Laboratory is performing a national-level study, funded by the EPA, on environmental endocrine disruptors. Endocrine disruptors are chemicals found in the environment that mimic hormones that control reproduction and other physiological processes in humans and other vertebrates. Environmental exposure to these compounds can have serious ecological and human health implications.
To accommodate projected growth in ecological restoration research and coastal security work, a new multiuse laboratory and office facility are proposed. The new facility will capitalize on the outstanding environmental assets of the location. More information about these proposed facilities can be found in Module 7.3.

**Bioproducts, Sciences, and Engineering Laboratory**

Our staff are developing innovative processes to convert biomass resources into higher-value chemical products and fuels. This will reduce the nation's requirements for petroleum and enable the economic viability of DOE’s biorefinery concept. To support these activities, PNNL and the State of Washington are working together to fund a new BSEL on the WSU, Tri-Cities campus. More information about this facility can be found in Module 7.3.3. Additional information about the Bio-Based Products and Processes program at PNNL can be found in Module 3.1.3.

To accommodate projected growth related to homeland security and coastal restoration activities, a new facility will be constructed at the Marine Sciences Laboratory in Sequim, Washington.
6—Research Management and Operations
6.0 Enhancing Research Management, Ensuring Operational Excellence

During the next five years, we will create new, distinctive capabilities for leading and managing a highly productive research enterprise.

Status

We have broken new ground and demonstrated strong leadership in improving both operational effectiveness and efficiency at the Laboratory. Our highly engaged staff, research and operational processes, and infrastructure are clearly working together to produce outstanding results for our customers.

- We received outstanding ratings in Laboratory Operations in four of the last five years.
- We increased our research productivity using an integrated management approach. For example, we have reduced overhead rates by 20 percent since FY 1994 while increasing our investment in scientific initiatives, staff, and facilities.
- The number of research staff as a percentage of total PNNL staff has risen each year since FY 1998, showing that more of the Laboratory’s funding is being directed toward research.

We are on track to maintain our record accomplishments through continued vigilance, revitalized approaches that keep staff energized around operational outcomes, and efforts to increase effectiveness and efficiency. With this strong foundation in place, we will invest in operations and new research processes to increase our research productivity.

Challenge

Our new methods of leadership in research management will improve our ability to turn discoveries at the frontiers of science into applications critical to DOE’s missions. Through managing our operations, we will improve our ability to leverage our people, processes, and infrastructure toward achieving higher levels of research productivity. New methods for improving research productivity will be focused both at the individual and the Laboratory level.

Plan

Becoming a leader in research management demands that we improve our core research management processes for understanding our customers’ needs, delivering high-value solutions, and stewarding the Laboratory’s assets. Starting at the Laboratory governance level (see Module 1.4), we must set clear performance expectations for these core research processes to 1) create more explicit and stronger linkages to the Laboratory’s strategies for integrating science and applied programs, and 2) translate S&T results into commercial applications. Because our staff use core
research processes daily, we will actively engage every staff member to help them understand these strategies so they can align their actions and decisions accordingly. We will use self-assessment as a means to improve our management systems. As we progress in aligning our actions and linking the core research processes with our strategy, we will accelerate our understanding of what is and is not working, and what actions are needed to stay on track toward our vision.

To meet this challenge, we must mobilize our substantial talent and resources in ways that will:

- Further integrate our management systems and develop more intuitive operational tools.
- Increase the levels of staff engagement by proactive communications, providing talented managers, developing staff, and providing competitive compensation.
- Strengthen the processes that link basic and applied sciences/engineering, starting with our Laboratory initiatives.

PNNL will continue to find new methods to better enable science while protecting the health and safety of workers, the public, and the environment.
6.1 Greater Research Productivity Using an Integrated Management Approach

We will improve operational performance in ways that increase our efficiency and effectiveness while enabling greater productivity of individual researchers.

Status

PNNL has a strong track record of outstanding operational performance, which includes:

- Reducing or holding steady the cost of operations while improving results that enable research.
- Obtaining highly respected external certifications, including those related to International Organization for Standardization (ISO) Environmental Management Standard 14001, the Voluntary Protection Program (VPP), and Integrated Safety Management (ISM).
- Increasing the extent that our staff are engaged in the functioning of the Laboratory. Our Gallup survey of staff engagement is showing steady progress in reaching levels maintained by the world’s highest-performing organizations.

Challenge

Our challenge is to provide revitalized approaches for continuing our outstanding record of safeguarding the Laboratory’s resources and protecting the health and safety of workers, the public, and the environment.

Plan

To meet this challenge, we will focus on the following key actions during the planning period:

- **Streamlining processes** will make additional resources available for reinvestment. By reducing low-value activities and finding ways to leverage new thinking and technologies, we can reduce the cost of administrative and operational activities to free up resources for investment of new infrastructure and capabilities.

- **Eliminating redundant, non-value-added requirements** is a powerful way to reduce the cost of administrative and operational activities. By eliminating unnecessary requirements, we can eliminate wasted effort and reduce cost while continuing to operate the Laboratory safely and efficiently.

- **Integrating operational and research processes** will allow researchers to spend more productive time on research. We will focus on improving our research processes to minimize the time technical staff spend on administrative activities so they can focus their energy on productive research. By embedding safety and compliance directly into the research processes, we can simultaneously meet both our operational and research objectives more effectively and efficiently.
**Maturing risk management and assurance processes** will allow us to increasingly use graded approaches to identify high-risk areas and establish appropriate risk limits. This requires a full understanding and definition of the key risks associated with achieving Laboratory goals and objectives. We will improve our approach to establish risk limits and metrics to monitor performance. Annually, we will brief the Battelle Laboratory Operations Committee (a corporate oversight committee) on our assurance results. To support this approach, we will evaluate our integrated management system to define which processes need to develop assurance plans that identify risk limits, self assessments, and other assurance resources, such as third-party reviews, that will ensure that management system objectives are being accomplished and that systems and controls are effective and efficient.

**Sharing lessons learned and best practices** across Battelle-affiliated laboratories will keep us informed of important process improvement opportunities. Although each laboratory is unique, many opportunities still exist to share and learn from the experiences of others. With a strong history of exporting management systems and tools to these other laboratories, we will continue to emphasize the value and benefits gained from sharing best practices and lessons learned with others.

**Safeguarding the Laboratory’s resources and protecting the health and safety of workers, the public, and the environment** will continue to be a priority. We believe that continued management vigilance needs to be coupled with renewed approaches that energize staff around operational outcomes.

The figure illustrates our concept of how the traditional support functions can be linked to form an integrated management approach that supports research and delivery of results. This integration effort is long and complex. We have made good progress to date, but we have several more years of developing and refining individual processes. The following modules (6.1.1 through 6.1.5) provide more detail on the performance of and our plans for the operation and financial management elements of our integrated management approach. Other elements are addressed in the modules highlighted in the figure.

- Environment, Safety, Health and Quality (ESH&Q)
- Safeguards and Security (SAS)
- Business Support Services
- Facilities and Operations

This figure identifies the major elements of the integrated management approach that we have implemented at PNNL.
6.1.1 ESH&Q Enables Research

Continued operational excellence at PNNL will be supported by ESH&Q enhancements that anticipate and respond to change while reducing both risk and cost to the Laboratory.

Status

Our ESH&Q program has a strong track record of outstanding performance that provides a firm foundation for building toward the future.

- Our sustained, outstanding ESH&Q performance is built upon customer focus, commitment to enabling research, and close cooperation with our DOE and PNNL customers.
- We met or exceeded DOE’s environment, safety, and health (ES&H) performance measures during the past five years.
- We received an outstanding rating in ES&H operations in four of the last five years.
- We achieved the ES&H Triple Crown, composed of highly respected external certifications including ISO 14001, VPP, and ISM.

Challenges

Our ESH&Q program faces two challenges:
1) finding and eliminating non-value-added process steps to improve efficiency, and 2) developing new software tools to enable research. The resultant savings will be used to invest in the renewal and revitalization of the Laboratory.

In parallel, we must continue to play a Battelle-wide leadership role in the continued enhancement of ESH&Q management systems and processes that anticipate and mitigate the risks affecting the Laboratory, the environment, and the surrounding community.

Plan

To meet these challenges, we will focus on the following actions.

- **Seamless integration of ESH&Q processes into Laboratory operational and research processes** is needed to support researchers without distracting them from research. Researchers will be able to spend more productive time on research by using tailored training and waste forecasting tools at the benchtop. We will deliver additional value-added tools that further integrate ESH&Q practices into Laboratory operations and research (e.g., enhanced Integrated...

- **Implement anticipatory risk management and mitigation tools.** We are planning ESH&Q system and tool upgrades that will anticipate and respond to risk in an environment of change. The new EPR and enhanced IOPS architecture will provide a graded approach that is integrated across all ESH&Q management systems and is transparent at the benchtop. The result will be the ability to anticipate and mitigate situations that would place the Laboratory in an unintended risk position, respond to project changes that would negatively affect our risk strategy, and manage the risk inherent in day-to-day operations.

- **Expand reliance on external requirements.** We continue to seek elimination of redundant, non-value-added internal or external ESH&Q requirements through the Requirements Integration and Tailoring process. External standards (e.g., Nuclear Regulatory Commission, Occupational Safety and Health Administration, and ISO) may be evaluated for applicability to Laboratory operations.

- **Streamline ESH&Q processes.** Work flow process techniques are being applied across management systems and PNNL Standards-Based Management System subject areas to identify specific interconnectivity improvements among work practices, information requirements, tools, and processes. To complement these efforts, we are working to improve the performance management processes used to monitor and inform us of our progress toward objectives, goals, and commitments. A new tool, PbViews, is being used to improve linkages from top-down strategies, connecting measures to strategies, facilitating timely decisions, and providing a consolidated source to determine if our performance objectives are being met. This effort will help us drive improvement in our processes and tools, minimizing their impact on research staff.

- **Ensure uniform ESH&Q management policies across Battelle-affiliated laboratories.** We are participating in the development and deployment of an ESH&Q Operations Manual that is based on the successful ESH&Q strategies, management systems, tools, lessons learned, and best practices developed across Battelle-affiliated laboratories.

PNNL will build on its tradition of operational excellence by using embedded tools and processes to increase research productivity.
6.1.2 Responding Appropriately to the New Threat Spectrum

PNL will enhance its Safeguards and Security program to respond to domestic and international events.

Status

- A broad risk-based approach for security management practices is used to determine protection priorities.
- Our Counterintelligence program complements and supports our SAS program’s risk-based approach by countering site-specific threats by foreign controlled adversaries.
- We worked closely with DOE to develop and implement local security upgrades (Security Condition [SECON] measures) in response to terrorist threats.
- We employ appropriate SAS measures to discourage or defeat attempts to collect information or disrupt operations by threats to scientific and technological information/programs.
- Our Cyber Security program evaluates emerging technologies and also adjusts its focus based on surveys, inspections, and self-evaluations.

Challenge

The Laboratory must find ways to quickly adapt to and effectively address changing SAS threats while minimizing impact to researchers and their work. In parallel, the SAS program must play a key role in mitigating risks affecting the Laboratory relative to the protection of information, and provide a secure but accessible environment that fosters research productivity.

Plan

To meet these challenges, we will focus on the following actions:

**Security processes and systems will be continually reviewed and enhanced.** To provide protection measures consistent with the national threat and homeland security advisory system, flexible, adaptive resources, systems, and processes to meet these evolving threats will be provided. SECON measures have been developed so DOE facilities would uniformly meet the requirements of the Homeland Security Advisory System and provide the appropriate responses and specific security upgrades for use under the different threat condition levels. We will continue to be responsive and take a proactive approach in the development and implementation of security measures to quickly adapt to and effectively address threats while minimizing impact to researchers.

**We will focus on information protection while keeping up with changing technologies.** A priority of our proactive SAS program is to employ appropriate measures that discourage or defeat attempts to collect information or disrupt operations by threats to scientific and technological information/programs. Our SAS strategy is to provide staff, collaborators, business partners, and customers a secure, but accessible, environment that enhances personal and team productivity through ready access to information, systems, and networks.
Strengthening and placing more rigors on the protection of sensitive unclassified information and cyber assets is key to the threat mitigation process. This increased emphasis will be accomplished in part through staff awareness and author accountability. As a result of expanding threats coupled with the increasing availability of information, another major focus will be the expansion of the Export Control program to identify and mitigate export control issues. Close interactions among SAS staff and the researchers will continue in order to understand and evaluate future access and protection needs.

We will pursue timely implementation of Cyber Security solutions. We will evaluate emerging technologies and potential applications to address the changing threats to communication and electronic information systems.

Our Cyber Security program evaluates emerging technologies and adjusts its security focus based on surveys, inspections, and self-evaluations. To address identified issues and vulnerabilities, we are providing near-term acceleration of the implementation of enclave architecture that will allow the differentiation of computing resources so that the appropriate level of security is applied based on risk and the work being conducted. Our Cyber Security program is also completing an upgrade to its primary Intrusion Detection System (IDS) to address all major traffic points. A firewall complex has been implemented to protect computing resources. A log review project that correlates information from numerous logs on the network including Firewall, IDS, Domain Servers, FTP servers, PKI servers, and web access is implemented, and additional analysis tools are being developed. A back channel network is also being implemented that will significantly increase the ability to manage the network securely and respond to incidents or threats more effectively. A software-based IDS using ZoneAlarm is also being instituted that will be installed on all systems that process sensitive information (Unclassified Controlled Nuclear Information/National Nuclear Propulsion Information).

Future solutions include development of a host-based (workstation) IDS that will continue to strengthen security of our individual workstations. A wireless rogue detection process is also being implemented that takes advantage of both the wireless and wired sides of the network. An IDS for our wireless network is also planned.

Several Cyber Security pilot programs are under way. Proximity devices for workstation access will be made available in the future for use where appropriate. An Instant Messaging Proxy server is also being piloted to allow better security and eliminate the peer-to-peer vulnerabilities. Additionally, a pilot will be run to determine the effectiveness of web appliances in the protection of web servers.

A cyber enclave architecture will allow the differentiation of computing resources in such a way that the appropriate level of security will be applied based on risk and the work being performed.
6.1.3 SAS Integration: Making Sure it Works

PNL is recognized as a model for integrating SAS into the line organization and operations.

Status

- The operating philosophy of PNL’s Integrated Safeguards and Security Management (ISSM) program was one of the first in the DOE complex. This program integrates SAS requirements into the processes of planning and conducting work at the Laboratory and assists management in addressing identified threats and associated risks. Our guiding principles as well as core functions of the ISSM program are reflected through the DOE policy that formalizes DOE’s philosophy for ISSM. Continued maturity targeted at performance-based security management is a current focus.

- The ISSM program has positively changed the security culture at the Laboratory. The role of SAS has shifted from enforcer to oversight and assistance, with implementation and the commitment to line organization accountability as essential. There is an increased awareness of security threats and risks as well as mitigation activities. Line organizations are now involved in the development and implementation of security requirements. Applicable research organizations are conducting monthly security assessments jointly with SAS staff. This ownership has led to a significant reduction in security issues and incidents.

- An Integrated SAS Senior Management Council has been established and chartered to provide a senior forum for the review of new and changing security conditions that affect the Laboratory, the identification of policy issues that should be raised to the leadership team, and the identification and/or endorsement of action plans as conditions warrant.

Challenge

Building a system that meets the needs of both science and security environments is essential, and the Laboratory must continue to evolve the maturity of the ISSM system to effectively accommodate both.

Plan

To meet this challenge, our SAS program will focus on the following actions:

**Continue the seamless integration of ISSM into Laboratory operational and research processes.** Continued emphasis of ISSM will strengthen security and ingrain it in the day-to-day activities of the line organizations.

Tools provided at the benchtop will support researchers by facilitating an open and supportive research environment coupled with an economical and effective protection strategy. Integration into Laboratory systems such as the new EPR, IOPS, and JETS will continue to be pursued. Our SAS program will employ performance management practices integrating planning and assessments using a performance agenda, assessments, and improvement initiatives as deployment mechanisms to
demonstrate the continual organizational learning process. Our SAS program will continue to concentrate on improving management practices, increasing productivity, and employing outcome-oriented performance measures to support operations contributing to the Laboratory’s success.

We will continue to identify and implement operational efficiencies, streamlining of requirements, and innovative approaches to facilitate effective security program performance while enabling productive research and minimizing costs.

Current enhancements to several SAS request systems included making them available from a single web page. The transition to the PNNL Digital ID as an electronic credential to be used for encryption, authentication, and digital signing was completed for these online systems.

Future enhancements include pursuing employee and nonemployee access to our SAS request systems from outside the firewall. A centralized role management and role-based access control service to define roles and capabilities within SAS applications will also be pursued as well as role-based Internet portal services and flexible ad hoc reporting tools to enable easier use of information. Also planned is more efficient (shared) use of individual system information (data warehouse concept) and interconnectivity between existing systems, the redevelopment of certain antiquated request systems on modern software platforms, and a defined migration for current SAS applications to the Laboratory’s predominant development platforms to minimize development and maintenance costs and increase staff productivity.

Sharing tools and best practices throughout the DOE complex. Collaboration with other DOE laboratories and entities will continue in the future to share best practices; enhance efficiencies across the DOE complex; and support development and implementation of effective and crosscutting protection strategies, security procedures, and measures.

Our SAS staff met with staff from ORNL and Lawrence Berkeley National Laboratory to share information about some of our programs such as the Foreign National Visits and Assignments; Foreign Ownership, Control or Influence; and Classified Matter Protection and Control. Material, procedures, and forms were provided as well as an offer to lend assistance in the future. Currently, SAS staff, along with our Information Sciences & Engineering group, are working with other Hanford Site contractors to deploy the automated Foreign National Visits and Assignments request system Site-wide.
6.1.4 Business Support Services at PNNL

Our culture will be to continually improve the reliability, usefulness, and timeliness of the information and services we provide with our staff. We will cultivate an environment of integrity, teamwork, candid communication, and professional inputs based on thorough yet concise information. We will encourage individuals to be proactive and innovative. We emphasize timely and effective support, not bureaucracy.

Status

We have achieved significant operational efficiencies in our business management systems to date. Recent examples include:

- Efficiencies from integrating acquisition and contract professionals with our business professional teams to realize synergies in capabilities as well as eliminate roughly $600 thousand in administrative cost.
- Web-based systems for inputting proposal pricing data, business planning data, procurement requisitions, and project risk data allow for reduced administrative effort in retrieving information and more accessible information for review both by PNNL and DOE at a detailed project level or aggregate Laboratory level.
- Master agreements with various vendors, leveraging the buying and travel volumes of Battelle-affiliated laboratories to negotiate significant cost reductions.

Challenge

The primary challenge facing our business management systems is maintaining adequate financial and compliance-based control while being responsive to the needs of our R&D environment. This requires easy-to-use systems and tools to allow projects and staff to proceed within the appropriate compliance envelope. Examples include inventory controls, cost reports, charging guidelines, funds controls, and acquisition processes.

Plan

A stable set of priorities guide our actions relative to adding value to our R&D environment while still meeting contractual requirements. We are planning several specific actions to address these challenges in our business management systems:

- We have a robust, compliant procurement system—our focus in the near future is to further our system through greater use of electronic commerce and web-based procurement mechanisms with master vendors, which will eliminate the administrative cost of multitudes of transactions.
- We will focus our attention on significant cost drivers as part of a cost productivity review to make $20 million to $30 million of resources available to reduce overhead rates and make necessary investments for the vitality of the Laboratory.
- We will facilitate an approach to prioritizing resources across the Laboratory based on the risk reviews started within the business management systems this past year.

- We will use technology changes to improve the value, quality, communication abilities, and timeliness of our business services while moving the Laboratory to paperless systems to the greatest extent practicable. We will continue to implement of electronic process improvements in the areas of electronic routing of invoices, electronic payment of suppliers, electronic distribution of cost reports, electronic submittal of time and travel reports, and other electronic interchanges.

- We will expand and strengthen ties with strategic small businesses to continue the process of establishing web-based catalogs for commodities that are repetitively purchased. Master agreements will be established with small businesses where possible, and large businesses will be encouraged to team with small businesses. We will partner with our key small businesses to identify and implement practices that represent a win for both PNNL and the small business.

PNNL will use commercial acquisition practices and leading-edge technology to develop a single connection between multiple Laboratory organizations and strategic suppliers.
6.1.5 Integrated Facility Asset Management

During the next five years, emphasis on decision-support processes for planning and executing facility maintenance and renewal, and integrating sustainable practices into facility operations will reduce the costs of operating and maintaining PNNL’s infrastructure.

Status

Our strong record of managing facility assets with distinction underpins future efforts for improving asset management practices. We have:

- Improved overall productivity by 35 percent and reduced cycle time by 67 percent through use of integrated and efficient work processes.
- Invested better than 2 percent of Replacement Plant Value on maintenance (includes maintenance bundled with general plant projects rehabilitation and improvement projects).
- Saved $500 thousand in annual energy costs through implementation of innovative tools, proven capabilities, and management approaches.
- Increased on-time delivery of planned jobs to above 95 percent.
- Attained more than a 99 percent on-time completion rate for preventive maintenance.
- Met over 13 percent of electricity needs from renewable power.
- Reduced energy use for laboratory and office buildings well ahead of schedule to meet DOE 2005 goals.
- Been recognized by the International Facility Management Association with the Golden Circles Award for outstanding facility management organization.
- Been recognized by the Federal Energy Management Program and Association of Washington State Businesses with multiple energy program and environmental awards for use of innovative approaches to conserve energy and reduce environmental impacts.

Challenge

We face two challenges:

- Increased attention by DOE on the management of its physical assets, including greater demand for accountability of assets and the call for long-term plans for maintenance and operation.
- Demands by management for overhead reductions, improved energy efficiency, and greater scientific productivity.

Plans

To meet these challenges, we will focus on the use of life-cycle analysis and long-term service life prediction processes, striking a balance between the risk of delaying maintenance against mission requirements and potential environment, safety, and health impacts.
We will **fully** integrate Risk-Based Life-Cycle Asset Management practices into our building operations and maintenance processes. Through these efforts, we will achieve mature implementation of commercial best practices for forecasting maintenance and renewal requirements based on industry standards spanning the life of a facility (typically 50 years).

Data collected from operations and maintenance activities will be routinely used by our system engineers to continually revalidate forecasted needs and to populate DOE corporate information systems, such as the Facilities Information Management System.

We will set maintenance investment levels to maximize operations of critical systems (electrical, HVAC, fire protection, etc.) in 300 Area buildings targeted for closure while deferring noncritical system maintenance unless required to meet mission commitments.

We will continue investment in energy management to achieve DOE's goals for energy reduction, maintain a diversified energy portfolio, and provide innovative low-cost solutions to infrastructure upgrades, where possible.

We will continue to acquire more than 10 percent of our electrical power needs from nonhydro “green” power, and will seek to qualify additional buildings to the Energy Star program and certify one facility as Leadership in Energy and Environmental Design – Existing Building.

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**Example of maintenance forecast processes at work for Building 326.**

![50-Year M & R Cost Summary](image)
6.2 Highly Engaged Staff

We are creating a working environment that enables S&T staff to develop exceptional credentials and outcomes, promote innovation and higher research productivity, and recognize technical leaders for their abilities to translate vision into action and align people and science challenges to DOE missions.

Best in Class

Research has shown that a highly engaged workforce is more productive than those that are less engaged, according to the Gallup Organization. We have assessed the level of engagement of our staff during the past two years by conducting a short survey, the Gallup Q12. The results of PNNL’s survey are analyzed against Gallup’s database to determine a percentile indicating our engagement score as compared to other research organizations. Our goal is to attain a best-in-class rating, which is defined as 75th percentile, for 75 percent of our workgroups, which indicates a highly engaged and productive workforce. We will continue to make regular and sustained progress toward achieving this goal; PNNL’s average has moved from 58 percent in 2001 to 69 percent in 2002.

Our practices are focused on creating an environment of highly engaged staff and managers who work with passion, drive innovation, and move the organization forward toward higher levels of scientific productivity. This includes a workforce characterized by staff members who are in roles that best suit their talents. We will continue to provide varied career path options and help staff identify their strengths, and then team them with great managers to create an engaging work environment.

Staff Development

PNNL staff identified the following areas for improvement: 1) providing more consistent feedback on progress and development, and 2) providing opportunities for staff to work in areas where they consider themselves the most talented. In response, we will create greater opportunities for staff to learn and grow by developing and implementing contemporary programs that facilitate staff growth. Our first step will involve working with a group of our most talented scientists and engineers to determine what specific development activities should be made available to our more junior scientists and engineers and developing a Scientist and Engineer Development Program to provide the tools and resources to enable staff development.

Compensation

We will provide effective total compensation programs that facilitate recruiting and retention of high-caliber staff and align performance with organization goals and outcomes. We have made significant progress in achieving a balanced compensation package of both base and variable pay programs, including programs focused
on recruiting, retention, performance-based reward and recognition, as well as targeted equity adjustments, as necessary. In the upcoming years, we will focus on transitioning from managing base pay to a total compensation market position involving extensive communication and training for both managers and staff. We will also monitor external markets to ensure that we maintain our desired market position and remain responsive to market trends. We will periodically review job family design to ensure that we are supporting organizational goals and outcomes with our compensation system design.

**Staff Communication**

We will provide staff communication and education through a variety of mediums to promote staff understanding, commitment, and ambassadorship for PNNL and DOE. We will accomplish this through progressive communications and marketing that targets delivery toward the audience experience level, interest, and availability. Priority will be given to staff interaction so that true dialogue and two-way communication are achieved. Retirees will be engaged through a specific retiree strategy that seeks to solidify and expand their ambassadorship as a strategic community resource. The desired end state for these engagements is an understanding and valuing of PNNL’s commitment to its diverse talent base of current and former staff.

Quartile Performance on Q12 GrandMean. More than 3 in 10, or 36 percent, of PNNL workgroups scored in the top 25 percent and are considered “Best in Class,” according to Gallup research.
6.2.1 Plans To Become an Employer of Choice

PNNL will become the employer of choice among those organizations conducting advanced scientific research, which will further our efforts to attract and retain exceptional researchers by providing exciting research opportunities and directions, outstanding research colleagues, a diverse workforce, a strong research community, and modern facilities and equipment.

Clear and Compelling Vision

By clearly communicating the compelling S&T direction of the Laboratory, our staff will help form and realize our vision and take pride in our impact. Through such avenues as this Institutional Plan, our strategic planning process, the Management Skills Development Program, and other forums, our leadership team will clearly express the significant scientific opportunities that are available to our staff.

Vibrant Workforce

We will ensure a vibrant and engaged workforce for the future through the delivery of integrated workforce planning systems and enhanced selection systems. We will increase our understanding of current staff demographics and capabilities and will target growth and selection decisions to ensure that workforce changes are made to meet our long-term objectives. By taking a comprehensive inventory of our available talent pool, identifying and providing growth opportunities to expand our current skill set, vigorously searching and hiring capable new talent, and planning for predicted business development, we will ensure future readiness to meet our needs. Where external talent is required, focused efforts will be made to attract the right mix of the best qualified individuals. The effectiveness of the selection and recruiting function will be measured for quality, timeliness, and efficiency.

Research Campus of the Future

We will provide a modern research campus that supplements EMSL with new user facilities and a campus of leading-edge equipment and research facilities. This will enable PNNL research staff and the broader scientific community to drive technical innovation and work on DOE’s most significant challenges (see Module 7.3.1).

Collaborations and Partnerships

We will draw upon our connections in the community to enhance our scientific collaborations and capability through partnerships with major research institutions in the region. These collaborations will enhance our research staff’s ability to deliver S&T to meet key regional and national needs, and will enhance the reputation of scientists and collaborative teams affiliated with PNNL. This will also create a pool of highly qualified and diverse candidates for employment at PNNL (see Module 7.2.3).
**PNNL Staff Population by Occupation and Degree Level**

(a) Data as of April 2003

<table>
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<tr>
<th>Occupational Codes</th>
<th>Total</th>
<th>Pct</th>
<th>PhD</th>
<th>MS/MA</th>
<th>BS/BA</th>
<th>Other</th>
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<td>Managers</td>
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<td>117</td>
<td>211</td>
<td>188</td>
<td>61</td>
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<td>S&amp;E/ Prof&amp;Eng/ SEA</td>
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<td>558</td>
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<td>Specialists</td>
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<td>189</td>
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<td>0</td>
<td>0</td>
<td>6</td>
<td>175</td>
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<td>0</td>
<td>46</td>
</tr>
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<td>763</td>
<td>772</td>
<td>1049</td>
<td>1268</td>
<td></td>
</tr>
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</table>
6.3 Enhancing Scientific Productivity: Researchers Doing Research

Access to high-performance instrumentation and computational tools, opportunities for collaboration with highly skilled coworkers, and an environment in which excellence is recognized and rewarded will promote a culture of productivity and excellence in scientific research.

PNNL must integrate different science disciplines to form effective, multifaceted, problem-solving teams. Our scientific productivity is measured by our success in achieving this integration of research capabilities. In addition to the conventional research productivity metrics (e.g., publications and intellectual properties generated) used in academia and industry, we must also consider metrics such as the degree to which information generated here is used in decision-making and deployment of discovery science to DOE problems. These outcomes can only be accomplished with quality staff, teamwork, the right tools and equipment, and a highly efficient infrastructure for performing research. This is enabled by creating the best environment for our scientists, and the ability for open communication of critical information for decision-making and creating the bases for technological applications.

Recognition

Peer recognition is an important factor toward ensuring that our S&T staff regard the Laboratory as an exceptional environment for their professional accomplishments and development. We must develop our staff into leaders of their fields and promote recognition by their peers—the ultimate individual metric for scientific productivity.

We will encourage our scientists to participate in high-level professional activities, such as serving in leadership roles in professional societies and participating in high-visibility working groups that provide leadership on important science issues. We will grow our staff through research opportunities on important science challenges and will communicate their findings through publications and appropriate forums, such as professional conferences and symposia.

To foster external recognition of key achievements among the scientific community, in 2003 PNNL implemented a Science and Engineering External Recognition program. Additionally, a new program for internal recognition for major scientific achievement is under development to enhance the previously established recognition program for major inventions by PNNL staff.

For our younger scientists, we must make resources available for them to test their ideas and enhance their career development. One current approach is the Fellows Initiative. Administered by the Council of Fellows, this program sets aside part of PNNL’s discretionary portfolio with the specific objective of encouraging the exploration of new concepts by junior staff under the mentorship of our most senior scientists and engineers.
Cutting-Edge Capabilities
Attract the Best and Brightest

Cutting-edge scientific capabilities, a highly competent staff, and a collaborative research environment are essential components to foster scientific productivity. We will sustain world-class scientific capabilities in our core disciplines to ensure that we are at the cutting edge in our signature areas. Simultaneously, we must create confidence that PNNL is working on high-impact science challenges and has the best tools and staff to do so in the DOE mission areas that the Laboratory supports.

To significantly impact important science challenges, we must be able to draw from our best talents across disciplines. Regional, national, and international collaborations with other leading scientists enhance the opportunities available to our staff, and complement and broaden our capabilities as a national Laboratory.

To encourage teamwork, we must consider new funding models and modern information technology infrastructure that will make it easier for our staff to have access to specialized experts and information across the spectrum of our research interests. Effective remote access to EMSL capabilities and enhanced connectivity to Internet II with the highest bandwidth available will create an environment that promotes exchange of ideas and thus enhance our ability to deliver high-quality science-based solutions to science challenges. This is an integral part of our research campus of the future and is absolutely essential for collaboration with the scientific community.

Efficiency Leads to Productivity

Rapid access to information using electronic libraries and databases; advanced computational methods for data storage, retrieval, and analysis; and assistance in theoretical modeling and graphical presentation of data are hallmarks of the most productive institutions. For significant scientific accomplishments, support should be made available to help our staff promote their findings to the appropriate audience, with minimal impact on time to our scientific staff. The goal is to increase the time for productive engagement of our best and brightest scientific minds.

Similarly, scientists must have the best tools available to conduct their best research. Breakthrough instrumentation and computational tools that advance the state of the art are the keys to scientific leadership in chemical and related sciences in this century. We must work with our sponsors to ensure that these scientific research tools are continually upgraded and readily available to the scientists. In turn, exceptional capabilities in the tools of science are essential to attract the kinds of collaborations that sustain PNNL in an S&T leadership role. These capabilities are exemplified in EMSL, and must be maintained at the cutting edge in capabilities for molecular science.

Our researchers have access to the state-of-the-art equipment, computational tools, and skilled experts necessary for conducting world-class research.
6.3.1 Transforming Scientific Knowledge into Information with Impact

PNPNL will optimize the impact of its primary product—information resulting from the conduct of research—through targeted enhancements in publishing and information management technologies and strategies.

Our publishing and library and information science professionals partner with researchers to support the entire life cycle of scientific and technical information (STI). In addition, we are now focusing on ways to optimize the impact of our STI—to strengthen PNNL’s reputation for scientific excellence and to maximize the benefits of investments in our publishing and information sciences infrastructure.

We will continue to expand our capabilities in areas that add quality and distinction to PNNL’s STI products:

- Graphics and multimedia, particularly three-dimensional animation, high-end digital photography, and digital video editing and production.
- Science writing for strategic audiences.
- Delivery of full-text electronic journals, bibliographic databases, and networked information repositories.
- Reference and research services.
- In-house workshop offerings on presentation skills, grammar, facilitation, accessible web design, and specialized information databases.

We will expand disclosure of and access to PNNL’s scientific and technical intellectual property by contributing original descriptive records for PNNL’s publicly available technical reports to national and international research databases.

We will add new value to information through advances in bibliometrics and content management strategies:

- Our publications, no matter how numerous, will not have impact if they are not read by the scientific community, potential clients, and other key audiences. We have begun to analyze the trends in our placement of articles in peer-reviewed research journals. Are our articles accepted in the journals that will most likely be read by those key audiences? Which journals might these be? STI professionals are teaming with senior research staff to find answers to these questions. Once we establish our list of “high-impact” journals, we can begin to target them, working with research staff to submit their work preferentially to...
these journals for consideration. Along with the list of high-impact journals, we will develop metrics to track our progress. Not only are we interested in publishing more articles in these journals, we want to see whether this will increase the number of times these articles are cited by others—one of the most tangible measures of impact.

*Our information is of little value to us if we are not managing it internally and leveraging it for reuse and decision support.* As the Laboratory begins to explore strategies for managing corporate knowledge, we are looking at ways to characterize and “catalog” the STI and operational information of the Laboratory. In looking at what other laboratories and companies have been doing, we are discovering that the most common mistake is a large investment being made in an information technology “solution” before the actual content is considered. We plan to start with the content: What is it about? Who uses it? In other words, what is the value of the information we propose to manage? Knowing this will help us design a content management model that merits the investment we make in it.

PNNL’s research is promoted by publication in top-ranked scientific journals and by employing high-quality multimedia to illustrate its breakthrough technologies. (December 2002 *Nature Materials* cover, with PNNL cover article, reprinted with permission from Nature Publishing Group.)
6.3.2 Information Resource Management Supporting Science and Research Productivity

PNNL aspires to be recognized by DOE as the model for applying and managing information technology to achieve the greatest possible value to clients, staff, and collaborators. We are aligning our information technology plans, investments, and information resource management processes to achieve this vision.

PNNL’s vision for information technology (IT) is to simultaneously excel at applying IT to solving the most challenging science and engineering problems, applying IT to managing and operating the Laboratory, and managing the information resources themselves. Attaining simultaneous excellence in these three areas requires that we achieve an appropriate balance among:

- The flexibility, ready capacity, high performance, and unfettered access sought by the open scientific community.
- The secure management of information resources that support our national security-related programs.
- The investments in IT to support efficient Laboratory operations versus investments in IT to enhance the scientific computing infrastructure.
- Achieving world-class efficient and effective management of information resources required by DOE, the DOE Office of Management and Budget, and Congress.

The challenges of simultaneous excellence are by no means unique to PNNL. Success demands creative problem-solving and outstanding relationships with the stakeholders—researchers and regulators alike.

A key element to achieving success in information resource management is our evolving IT planning framework. This framework consists of three parts:

1. **IT Strategy** - provides a high-level roadmap of how IT investments and information resource management activities will be aligned to help accomplish our mission and vision and support specific research activities and management system needs.

2. **IT Architecture** - describes in greater detail the current state and target state of our IT environment and the technology standards to be applied.

3. **IT Investment Portfolio** - refers to the total of our information resources and IT investments. The term “IT portfolio management” refers to the business processes used to select and monitor investments in IT and to prevent redundancy of existing or shared information resources.

Information resource management at PNNL relies on close cooperation and participation among Laboratory leadership, the research directorates, and management system owners to develop, approve, and maintain these plans.
The IT strategy process is well established at PNNL with annual updates to the plan made since FY 1997. In FY 2002-2003, we invested to refresh our IT architecture document and to implement processes to keep this tool up to date. In FY 2003, we instituted a Program Management Office to monitor IT investments and provide project management support to general IT infrastructure and business information systems projects, and began to investigate best-in-class processes and automated tools for portfolio management. In FY 2004-2005, we will institutionalize the IT portfolio management processes that best fits the Laboratory's culture and other business processes, and implement automated planning and tracking tools to reduce the administrative burden.

The following key desired business outcomes from IT investments at PNNL were identified or confirmed through the IT strategic planning process for the FY 2004-2008 planning period. At the top of the list are those that are central to supporting the science mission of the Laboratory, followed by those that promote leadership in research management and operations.

**Outcome 1:** Support valued research programs that demand high-performance information resources.

**Outcome 2:** Provide research and support staff with reliable and cost-effective access to needed information resources, regardless of location.

**Outcome 3:** Foster innovation and improve problem-solving through collaboration.

**Outcome 4:** Increase individual and work group productivity.

**Outcome 5:** Reduce the life-cycle cost of information technology.

**Outcome 6:** Reduce the burden, cycle time, and cost of administrative processes.

**Outcome 7:** Provide better information and tools for proposal, project, and capability management.

PNNL's IT planning process aligns IT investments to Laboratory objectives and priorities, promotes efficiency through technical standards and by eliminating redundancy, and monitors IT project and service performance to quickly identify potential problem areas.
6.3.2.1 Fostering Scientific Discovery and Innovation Through High-Performance Computing

Access to high-performance computational resources—computers, information stores, and specialized software—is essential to strategies in all PNNL research areas. The initial single-mission high-performance computational focus realized in the Molecular Science Computing Facility is being broadened to support an increasing number of smaller missions requiring high-performance computing resources for scientific discovery and analysis as well as engineering models.

PNNL’s scientific and technical computing needs are driven by a variety of missions. High-performance scientific and technical computational support is critically important to our initiatives and ongoing research in biology and environmental and computational sciences, including those supported by the existing EMSL user facility and the future the DOE Genomics:GTL Facility II, the Whole Proteome Analysis Facility. The Laboratory must also be positioned to support other valued research programs, such as those related to energy and environmental S&T, that are unable to purchase dedicated large-scale computing and data storage resources. Finally, access to classified high-performance computing resources is essential to our important contributions to the DOE National Security mission and our expanding role supporting the DHS.

Our scientific and technical computing strategy is a partnership among the Molecular Science Computing Facility (MSCF) (housed within EMSL), the Computational Sciences & Engineering Initiative (CS&EI), and the Information Resources Management System (IRMS). Combined, these three entities deliver high-performance computing resources, large-scale data storage facilities, and specialized software tools to PNNL researchers and collaborators.

World-class computational resources housed in the MSCF are available for basic and applied research in environmental molecular science. During FY 2003, the MSCF installed an 11+ teraflop Linux-based supercomputer from Hewlett-Packard. The system has 1900 Itanium-2 (Madison) processors with 7.8 terabytes of system memory and 253 terabytes of I/O storage. The computer is available for both Computational Grand Challenge Projects and smaller general research projects.

The CS&EI (see Module 2.4.1) was established to strengthen PNNL’s core capabilities in computational science, build program depth with the DOE’s SC Advanced Scientific and Computational Research, and drive new classes of high-end modeling and simulation that significantly advance understanding in the physical and biological sciences. To support this strategic intent, CS&EI has implemented a 0.3-teraflop cluster computer that is available through an internal proposal/review process to provide compute cycles to major research areas across the Laboratory including subsurface modeling, biology, engineering, climate modeling, chemistry, homeland security, and other mission-critical areas.
In the next few years, the MSCF and CS&EI expect to expand their approach to high-performance computing to include tightly coupled but widely geographically distributed computing and data storage resources at other laboratories and institutions. This poses significant challenges. First, this approach will require greater bandwidth and lower latency in our Internet connectivity than is delivered by ESnet today (described further in Module 6.3.2.2). Second, we must work with our peer laboratories and DOE to resolve cyber security-related policy issues and technical challenges to establish seamless multi-institutional resource interconnectivity.

Few programs can justify and afford computational resources of the class of the MSCF. To better support valued research programs that are unable to purchase dedicated high-performance computing resources, the IRMS is working with the MSCF and CS&EI to implement and promote ways to effectively aggregate and share computational resources across programs to build larger general-purpose computing capabilities. We will continue to provide and enhance network access to shared high-performance computing resources located at other sites and facilities, such as the National Energy Research Scientific Computing Center. We intend to supplement those offsite resources by implementing capabilities locally that facilitate pooling of computing resources between smaller programs and projects. In FY 2004, we will implement a general-use Linux-based cluster computing resource by reallocating an available interconnect switch. Projects will be able to join the cluster for modest costs and add capacity in small, affordable increments. A second general-use cluster will be added in FY 2005 to support Windows-based applications.

Another way we will facilitate pooling of resources is through a subscription-based service that provides our researchers access to a broad collection of scientific and technical software tools through a centrally managed, concurrent licensing system. Introduced in FY 2002, this service has proven to be very popular with PNNL researchers and a cost savings to sponsors. We will continue to expand this service by annually adding new applications and expanding existing licenses to meet increasing demand.

Computing support for PNNL’s classified work is provided using desktop workstations housed in Limited Access Areas and a secure computing facility (SCIF). The computational needs of our classified work have evolved to far exceed the space within these resources. We are taking a two-pronged approach to providing researchers with access to classified high-performance computing resources: 1) classified network access to resources located at other sites, and 2) a local classified high-performance computing cluster. Initial capabilities for both were implemented during FY 2003 with connection to a single-mission classified network and installation of a cluster computer in our existing SCIF. In FY 2004 we will implement connections to additional mission-specific classified networks. Requirements for additional classified computing room space are being included in the planning for new facilities.
6.3.2.2 Network Connectivity: A Key Enabler and Critical Challenge to S&T Excellence

Although PNNL has greatly improved network connectivity over the past two years—benefiting the Laboratory as well as other regional research and education institutions, local businesses, and Tri-Cities residents—significantly greater bandwidth is needed to support biology and national security research initiatives.

Improving PNNL’s network connectivity is critical to establishing the new Whole Proteome Analysis Facility for the Office of Biological and Environmental Research (BER) and to making other significant contributions to SC multidisciplinary, multi-institutional research programs. Projections by researchers indicate immediate need for OC12 (622 megabytes per second [Mbps]) Internet bandwidth, increasing to at least OC48 (2.5 gigabytes per second [Gbps]) by the end of FY 2005. A minimum of OC192 (10 Gbps) Internet bandwidth will be needed to replicate massive experiment datasets to multiple collaboration sites when the proteomics facility comes online in FY 2007. In addition, implementing classified network connectivity is essential to our contribution to the DOE National Security mission and our expanding role supporting the DHS.

We are investing in network improvements to meet many of these needs. In FY 2002, we improved internal network performance by upgrading our backbone with switches capable of handling multiple 10-gigabit Ethernet paths between facilities and started to deploy 1-gigabit Ethernet to individual offices and laboratories. In FY 2003, our firewalls and border routers were upgraded to accommodate increased bandwidth to the Internet. Working with local businesses and Internet Service Providers, we have established a Local InterNetwork eXchange to keep local traffic local and provide better Internet service for PNNL, other local businesses, and Tri-Cities residents.

Providing sufficient Internet bandwidth for communications with research partners is a particular challenge due to the relatively high cost of bandwidth to eastern Washington State. Until mid-FY 2003, PNNL network connectivity with DOE, university, and industrial research collaborators was provided exclusively by an OC3 (155 Mbps) connection to ESnet. Our path for connectivity was an OC3 circuit to the Pacific Northwest GigaPOP in Seattle, funded from PNNL general and administrative overhead, and an OC3 connection from the Seattle GigaPOP to the ESnet “cloud” funded by SC. We also funded a low-speed (1.5 Mbps T1) backup path to the Internet to provide connectivity for business-essential applications during rare interruptions to ESnet service.

In FY 2003, we increased bandwidth to university research partners fourfold by upgrading our connection to the Pacific Northwest GigaPOP to OC12 and joining the Internet2 Abilene network. We also upgraded our backup path to the Internet to 10 Mbps using a commercial Internet Service Provider. By leveraging and supporting the efforts of public utility districts who are working to extend broadband network service to rural communities in Washington State,
and by partnering with CalTech and the National Science Foundation-funded Hanford Laser Interferometer Gravitational Wave facility, these improvements have been made with very little increase in operational costs and no impact on PNNL general and administrative rates.

Despite these improvements, network connectivity to research partners at other DOE laboratories is still constrained by the OC3 ESnet connection with the Seattle GigaPOP. BER program support is needed to overcome this bottleneck and increase the ESnet circuit to at least OC12 in FY 2004, consistent with our connection to collaborating universities, and to OC48 by the end of FY 2005.

Finally, we are actively exploring options for even greater bandwidth, both within and outside of the region, to support the Whole Proteome Analysis Facility and other research programs. Multiple alternatives are available. NoaNet, which currently supplies our OC12 connection to the Seattle GigaPOP, is capable of supplying OC192 bandwidth to Seattle and Portland, where we can connect with ESnet and Abilene through one or more national telecommunications carriers. The National LambdaRail, a fiber optic research network being constructed by a consortium of universities, will pass within 30 miles of PNNL’s Richland campus (see the figure). This network is capable of delivering multiple 10 Gbps wavelengths (Lambdas) to serve very high-end experimental and research applications. The ESnet technical strategy includes moving to an owned fiber-optic network similar to the National LambdaRail. Level3, the company providing fiber optics to the National LambdaRail, can also provide fiber optics to ESnet to provide connectivity to PNNL as part of future upgrades.

PNNL is initiating an effort among the DOE laboratories to define near-term and long-term network bandwidth requirements for biological research and represent these unmet needs to the ESnet steering committee.
6.3.2.3 Increasing Individual and Team Productivity Through IT

PNNL’s plans for personal computing and collaboration technology for the next few years are evolutionary, not revolutionary, and are focused on reducing total cost of ownership, while continuing to increase the functionality of tools available to our staff to improve scientific effectiveness and productivity.

Driven by our tradition of cross-disciplinary research as well as our geographic location, PNNL has long been a leader in deploying and using IT to increase the productivity of dispersed teams. “A Laboratory Without Walls” was a strategic theme at PNNL as early as 1992, and the concept of a “collaboratory” was prominent in early proposals for EMSL.

Today, our innovative electronic collaboration and information-sharing tools enable diverse teams of staff and collaborators to work together, irrespective of time or location, to deliver the maximum possible value to our customers. Our staff have ready access to a rich pallet of collaborative tools that enable more effective and efficient conduct of research and operations functions. Capabilities in use today include:

- Extensive videoconference facilities (fixed conference rooms, mobile units, and high-quality desktop systems).
- Two nodes on the worldwide Access Grid for multisite meetings and research collaborations.
- WebEx™, a commercial service for remote meetings, presentations, and demonstrations of research products.
- CollabraSuite, a collection of tools for team information-sharing, brainstorming, task tracking, discussion groups, and virtual meetings.
- CORE2000, a real-time Internet collaboration environment developed for EMSL that includes audio, video, whiteboards, shared applications, and remote instrument access.
- Electronic Laboratory Notebook, a web-based system for individual or joint authoring and recording of research activities and results.
- Broadcast of live and recorded meetings and presentations over the PNNL intranet (see the figure).
- Electronic mail featuring Entrust-PKI encryption for privacy of communications with DOE and other DOE laboratories, and effective spam controls and virus protection.

These tools allow for capturing and sharing of information, joint authoring of documents, brainstorming over long distances, and electronic meetings that reduce the cost, lost productivity, and personal “wear and tear” of travel.
Our actions in the next few years are focused on delivering the highest possible value returned from the Laboratory’s $7+ million annual investment in personal computing equipment, software, and services. Our strategy is to lower the life-cycle cost of ownership through standardization, configuration management, electronic procurement, leveraged purchasing deals, and concurrent user software licensing. We will simultaneously improve the productivity of IT users through convenient and cost-effective support and training, including online, “just-in-time” training on commonly used software. We will continue to enhance and expand the core collaboration tools and capabilities, and replace custom-built tools with cost-effective commercial equivalents as they become available. We will expand use of the Internet as a ubiquitous and cost-effective communications transport. For instance, in FY 2004 we will begin to pilot Voice-Over-IP in place of POTS—“plain old telephone service.”

Finally, and most importantly, we will aggressively educate and train our research staff on the availability and use of IT to increase their productivity, empower effective collaboration with other DOE laboratories and regional universities, and continue to leverage PNNL’s strength in interdisciplinary research.

Researchers can view and participate in guest lectures, briefings, and meetings broadcast live over the PNNL network using streaming video technology. This allows broader participation by staff, regardless of their location. Broadcasts can be recorded and replayed on demand by travelers or other staff who are unable to view the event live.
6.3.2.4 Enabling Operational Excellence Through Business Information Systems

The focus of PNNL investments in business information systems has shifted from increasing IT efficiency to optimizing business processes. The result will be even greater research staff productivity and contributions to PNNL leadership in research management.

During the past five years, we have worked diligently to increase the value of IT to managing the Laboratory by implementing information systems that improve the efficiency and cost effectiveness of vertical business processes housed within the Laboratory's management systems, and that assist staff to protect the environment, ensure public health and worker safety, and comply with regulations and policy. We have adopted an industry best practice of incrementally implementing and integrating commercial off-the-shelf business information systems. However, when there is no appropriate commercial solution or solution developed at other federal laboratories, we have the capability to develop our own best-in-class business applications. Some of these custom applications have been adopted by other federal research facilities, and others have been commercialized. Our Chemical Management System, Assessment Tracking System, and Standards-Based Management System have all been transferred to other DOE and DoD sites. In addition, the Chemical Management System and our Purchase Card applications have been sold commercially.

We have also strived to increase the efficiency of business information systems implementation, maintenance, and operations by reducing complexity through standardization and by implementing a mature data warehouse environment that is used to capture, share, and preserve information, and to efficiently integrate business applications. This effort is a work-in-progress with changes made to existing applications only in the course of normal system life-cycle upgrades, but significant progress and favorable comparison has been noted as a benchmark of PNNL IT conducted by the Hackett Group.

In the next several years, our investments in business information systems will shift focus from improving IT efficiency to optimizing business processes, as represented in the figure. This shift will include investments in three areas: business applications, business computing infrastructure, and business data management.

Business Applications

As previously noted, we have worked diligently to implement information systems that improve the efficiency and cost effectiveness of vertical business processes housed within the Laboratory's management systems, and that assist staff to protect the environment, ensure public health and worker safety, and comply with regulations and policy. The next evolution of PNNL business information systems are role-based workflow applications that contribute to seamless integration of management system processes—reducing the burden on researchers and enabling them to spend even more of their time on research while continuing to safeguard the Laboratory's resources and protect the health and safety of workers, the public, and the environment.
Business Computing Infrastructure

For the past several years, we have worked to simultaneously reduce the cost and improve the performance and reliability of our business computing infrastructure by reducing complexity. With measured success in that effort, our focus has shifted to adding the infrastructure capabilities needed to seamlessly integrate existing and future business applications as described earlier. Specific capabilities being implemented now and during the next few years include a role-based access control system, an application integration workflow engine, and an intranet portal environment.

Business Data Management

We have a very mature data architecture that supports business transaction processing and decision-making. This architecture incorporates a data warehouse that captures and stores historical transaction data, an operational data store that is used for integrating business applications, and “data marts” that are optimized for online analysis and reporting of business information. Benefits from investments in this architecture have included improved project financial performance due to the delivery of more timely and complete cost information, better management controls through the ability to audit and analyze transaction data, and reduced business application development and integration costs. Current efforts and future plans will improve the sharing of operational data using web services and will add content management functionality for capturing and sharing research capabilities, best practices, proposals, and other similar unstructured information.

Investments in PNNL business information systems have shifted focus from increasing IT efficiency to optimizing business processes. The result will be even greater contribution to PNNL leadership in Laboratory management.
7—Community and Stewardship
7.0 Plans for Community Engagement and Stewardship

PNL will play a significant role in building a vibrant economy and fostering a business climate and quality of life that will not only ensure its long-term success, but that will bring significant benefits to the community and the Northwest.

In the next five years, we will enhance our commercialization program, generating returns for the Laboratory as well as our region. Our experience in serving both private and government markets enables us to transform scientific knowledge into useful products that will benefit the economy and society. Success in technology commercialization begins with our staff, who will be engaged in strategy development and rewarded for their efforts in developing intellectual property. We also are looking for partners who can help us deploy technology—partners who understand the market needs and who might be willing to co-invest in maturation and product development. Through an effective commercialization program, we can reinvest in the Laboratory's staff and infrastructure, making it an even stronger S&T asset for the region and the nation.

Beyond the Laboratory's own commercialization program, we will be linking the substantial S&T resources of the Northwest. PNL and its partners intend to create new products and services that will spur economic development. One program, called Linking Regional Resources, is aimed at identifying promising new technologies from a pool of intellectual property garnered from several key research organizations. Our Technology Entrepreneurship Program then takes the next steps of evaluating the commercial potential of the technologies and developing business plans and a path forward. Based on the data and outcomes produced from these first two efforts, PNL's New Ventures Program seeks to establish successful commercialization ventures.

We also will be using new approaches to grow and attract technology-based business that shift the local economy from its current dependence on Hanford Site cleanup programs. By making our researchers available to regional businesses for a limited time at no charge, we can provide much-needed technical expertise in a wide range of fields. We are helping entrepreneurs connect with funding and business expertise as they make their way through the typically long gap between product invention and revenue generation. In addition to assisting existing and new businesses, we are leading an effort to attract the research operations of large corporations to locate near PNL. And because of our connections to technology business advocacy organizations, we can provide information critical to technology-based entrepreneurship.

We recognize that our role in strengthening the local and regional economy is only one part of the definition of good community stewardship. We are looking beyond the R&D needs of the region to needs of the future workforce—the young women and men who bring us the next-generation breakthrough S&T. Through a wide range of workforce programs for students and teachers, we will
help ensure that there is a sufficient pipeline of qualified scientists and engineers. For example, we plan within the next two years to be fully participating in the Laboratory Science Teacher Professional Development program, a new DOE initiative designed to support teacher quality. We will continue to be a key partner in improving science education through the Washington State Leadership and Assistance for Science Education Reform project.

Underlying our success at increasing PNNL’s impact on regional economic development and quality of life is our ability to continue working at the frontiers of science and technical innovation. During the course of the next five years, we plan major acquisitions and modifications to our research campus so we can effectively address DOE’s most significant challenges and contribute to the vitality and prosperity of the community and region. Our plans for modernizing our research campus call for relocating out of the 300 Area to support Hanford Site cleanup; replacing aged, Cold War 300 Area facilities that house core research capabilities; establishing key partnerships that expand our capabilities through shared staff, equipment, and facilities; and acquiring new user facilities that strengthen the regional S&T base.

PNNL has long been known for being a good community steward and a partner in local economic development, but we recognize that it is time to expand the Laboratory’s S&T resources to make a more significant contribution to the region. Through the efforts outlined above, we envision that PNNL will set the standard among DOE national laboratories for creating and deploying technologies that advance economic prosperity and community vitality.

PNNL’s Model for Community Engagement and Stewardship shows how enhanced efforts ranging from technology commercialization to science and engineering education, coupled with strong volunteer programs and generous corporate donations, will strengthen PNNL’s presence and impact both locally and regionally.
7.1 Reinvesting in the Laboratory Through Technology Commercialization

Through a strategic Technology Commercialization program, PNNL will provide high value to our partners, society, and the economy, and generate returns that will be reinvested in the Laboratory’s staff and infrastructure.

Battelle brings a long history of commercial experience combined with distinguished performance in the management of PNNL. Our experience with private industry and private capital markets and partners, as well as the government, allows the dual objective of advancing scientific knowledge and converting that knowledge to useful products in areas of commercial market interest. Through successful commercialization and technology deployment, revenues are reinvested in staff and infrastructure, enhancing and strengthening the R&D capabilities of the Laboratory.

Our Technology Commercialization program will strategically capture, evaluate, protect, mature, license, and manage PNNL-developed intellectual property to assist in growing DOE, other government, and commercial business at PNNL. Intellectual property experts focus on early and frequent engagement with technical staff, knowledge of current programs and projects, and shaping R&D toward high-value outcomes. We combine invention evaluation and positioning with early business information and market characterization to assess the benefits of protecting or maturing intellectual property derived from R&D programs. Using a combination of patenting and business management skills, we will provide efficient patenting decisions and results. Technical staff will be engaged in the strategy development and commercialization process and be rewarded for their intellectual property development and commercialization results. A broad array of appropriate government and private resource investments are applied in promising technologies to maximize the value for deployment.

Deployment options are broadly evaluated to include balancing commercial opportunities with contract R&D at all stages. We will identify key strategic partners for licensing and business development for future growth and revenue generation. Priority consideration is given to investments where knowledgeable partners understand the market needs and ultimate product success criteria, and are willing to co-invest in maturation and product development. We will deploy Laboratory technology and intellectual property through a variety of technology transfer mechanisms appropriate for both the partner and the Laboratory. Experienced licensing professionals are assigned technology portfolios that are actively marketed. We use best practices in a variety of ways to offer the best tools available to conclude successful licenses.
Commercial success will provide recognized infusion of DOE S&T into the public economy, demonstrating to Congress and the public that DOE’s programs are a good investment of taxpayer dollars. Reinvestment of commercial returns will provide resources for science, technology, and capability development to meet future DOE and national needs. We will continue to apply our revenues from privately and DOE-funded technology transfer activities to fund new capabilities, new equipment, and R&D in DOE and Battelle-owned facilities at the Laboratory to seed next-generation technologies. Investments by Battelle in technology maturation, product development, patenting, and licensing activities at PNNL will significantly enhance the value of DOE-derived technologies. The ultimate payoff is in creating and deploying technologies that advance science, create new knowledge, and benefit the economy and society.

Value Creation Wheel – PNNL’s Technology Commercialization program fosters strategic technology deployment through commercial licensing or other technology transfer mechanisms. Benefits such as increased public knowledge, new companies and products, and reinvestment revenues are realized.
7.2 Major Economic and Educational Benefits to the Community and Region

PNNL will contribute to an economically vibrant and diverse community and region through its S&T resources, robust workforce development pipeline, and Northwest partnerships.

Linking Regional Science and Technology Resources

We will achieve Northwest social and economic development objectives by linking the S&T resources of the region’s major institutions. The region’s public research institutions collectively conduct over $2 billion in R&D, which in turn produces valuable intellectual property and technical capabilities that can be used to solve social and industrial problems in the Northwest. In collaboration with government and trade organizations, we have formed the Linking Regional Resources group, which identifies areas where technologies can address issues of concern to the Northwest. Further, by working with the university technology entrepreneurship programs, investors, and entrepreneurs, PNNL—along with its partner institutions—can form viable business solutions that not only help to strengthen the economy, but also address the technology-based needs of the state’s and regional industry. See Module 7.2.1 for discussion of specific planned activities.

Local and Regional Growth and Diversification

We will grow and diversify the local economy by using our technology resources and network relationships. The overall objective is that the local and regional technology-based economy will be significantly more diverse, with PNNL having served a meaningful role in creating that shift. We will devise new economic development approaches, while also using proven approaches, to help grow the technology sector. We will make our researchers available to regional businesses for limited engagements at no charge while striving to achieve a high level of client satisfaction, as measured by surveys. Using our connections throughout the Northwest, we will play an important role in helping local and regional firms obtain the necessary investment and grant funding for new product development and company growth. We are also undertaking an effort to attract other large technology-based organizations to the local area. Finally, we will create and provide information to help entrepreneurs access money, business opportunities, experienced management team members, and other sources of expertise. See Module 7.2.2 for discussion of specific planned activities.
Science and Engineering Education

We will enhance the S&T pipeline and support economic development by improving regional science and engineering education. Our programs integrate research and education and will link the Laboratory’s human, financial, and technical resources with elementary and secondary schools, colleges and universities, and other education-oriented organizations to improve learning and teaching. Activities will include 1) promoting and facilitating research and education partnerships with postsecondary institutions, 2) enhancing S&T literacy of students and teachers, 3) contributing to the education of future scientists and engineers, 4) promoting diversity in the science and engineering “pipeline,” 5) connecting academic learning to the world beyond the classroom, and 6) providing an education forum for discussing science issues. See Module 7.2.3 for discussion of specific planned activities.

PNNL will contribute to a technology-based regional and local economy by providing S&T resources, a robust workforce development pipeline, and partner relationships.
7.2.1 Building Substantive Partnerships and Regional Advocacy for PNNL and DOE Missions

Through three key programs—Linking Regional Resources, Technology Entrepreneurship, and New Ventures—PNNL connects its S&T resources with those of the region’s major research and business institutions, thereby achieving its Northwest social and economic development objectives.

Linking Regional Resources

PNNL, through its Linking Regional Resources (LRR) program, partners with major research institutions in Washington, Oregon, and Idaho to identify, link, and provide technology solutions that address regional social and economic development objectives. This program, established in 2001, collects, analyzes, and bundles the Northwest region’s intellectual assets. The goal is to use the intellectual property to create new products and services, thus stimulating regional economic development and enhancing quality of life. Potential applications of the S&T inventory created via LRR include coastal and homeland security, environmental protection and cleanup, enhanced power distribution, bioproducts and bioprocessing, and more.

In most cases, technologies are viewed as viable, but do not always have a clear path to market. Regularly, patents and related information provided by the participating research organizations are entered into a PNNL-developed information visualization software called Starlight. The software compares the entire inventory of intellectual properties, identifying and bundling together similar technologies that may be more effective, versatile, and valuable when applied collectively.

During the next five years, we will continue to regularly gather and analyze the intellectual properties provided by partners. Additionally, we will strengthen our relationships with participating regional institutes, foster innovative collaborative approaches to commercialization, and reach out to new potential members. Current members of LRR include senior representatives from the research and/or technology transfer offices of the INEEL; the Oregon University System (Oregon State University and the University of Oregon); the Inland Northwest Research Alliance (WSU, Idaho State University, and the University of Idaho); the Oregon Health & Science University; the Fred Hutchinson Cancer Research Center; and the University of Washington.

Technology Entrepreneurship

While identifying technologies to solve specific problems is important, it is not alone sufficient to move the technology forward to provide a benefit in the marketplace. PNNL’s Technology Entrepreneurship program uses the region’s matriculating entrepreneurial students to develop commercialization strategies for promising intellectual properties.
The Technology Entrepreneurship program examines technologies from PNNL and other major research institutions, evaluates the commercial potential of the technologies, and develops strategies for commercialization, including business plans that identify the pathway, steps, and resources required. Through this program, we are forging strong partnerships with colleges and universities aimed at both commercializing promising technologies and, perhaps most importantly, developing the entrepreneurs of tomorrow. We have worked successfully with the University of Washington and the University of Oregon to provide opportunities for business students to formulate business plans for promising PNNL-developed technologies. Some of the plans have received awards in national competitions. In the future, the program will build on existing partnerships and broaden the capability by cultivating new programs with other regional universities.

**New Ventures**

The third element in PNNL's regional approach, the New Ventures program, seeks to create significant value for the Laboratory and region by establishing or expanding new high-technology enterprises in the Northwest. New Ventures is designed to translate the data and outcomes produced by the LRR and the Technology Entrepreneurship programs into successful commercialization ventures. For technologies possessing promising commercial potential, solid market and strategic business information, and seasoned management teams, the New Ventures program moves intellectual properties from the strategy and planning stages to the marketplace via a network of Northwest business experts and organizations. The technologies will come increasingly from the bundles of intellectual property created by the LRR program, and the university entrepreneurship centers will provide the market and strategic business information. Networks of entrepreneurs and managers will provide the required management skills.

Through these various programs, we are harnessing our breakthrough S&T to achieve excellence and accomplish key DOE goals, including:

- Delivery of S&T to meet key regional and national needs.
- Promotion of regional research collaborations that maximize the value of research dollars and discoveries.
- Development of new businesses, which will lead to regional economic development and diversification, as well as enhancement of the Northwest's quality of life.
- Creation and sustenance of innovative entrepreneurs who, over the next 20 to 50 years, will find effective new approaches for moving technology from the laboratory to the marketplace, ensuring that over the long term, PNNL delivers tangible, real-world solutions to the region and nation.
7.2.2 Applying PNNL’s Technology Resources to Diversify and Grow the Local and Regional Economy

PNNL will apply its technology resources and connections to grow and diversify the local and regional economy, playing a meaningful role in the transition to a technology-based sector that is significantly less dependent on Hanford Site funding.

Economic Development and Diversification

We will use new economic development approaches to start, grow, and attract technology-based businesses locally. The overall objective is that the local technology-based economy will be significantly less Hanford-dependent, with PNNL having served a meaningful role in creating that shift. The Three Rivers Technology Alliance, which PNNL leads, is currently developing specific goals to assess progress toward a technology-based, Hanford-independent local economy. These goals will serve to guide our efforts to diversify and grow the local economy. We will devise new economic development approaches, some described in the following sections, while also using proven approaches, to help grow the local technology sector. The new approaches will be used to obtain funding for entrepreneurs, recruit experienced executives for entrepreneurial ventures, and develop a “critical mass” of technology-based employers in the local area.

Providing Technical Assistance to the Community

We will make our researchers available to regional businesses for limited engagements at no charge. While PNNL offers more than a dozen economic development programs, one of the most impactful is the Technology Assistance Program, in which researchers are made available in one-week increments to provide technological help to businesses upon request at no charge. We will strive to continue to deliver this program with satisfaction rates exceeding 90 percent, equaling the results achieved while providing assistance to about 600 firms during the last 8 years. While purely demand-driven, we will continue to provide technical help in areas such as new product development, materials characterization, chemical process development, peer review of new technologies, environmental management, medical devices, software design, energy conservation and production, and advanced sensors.

Finding Funding

We will help make regional business experts and funding sources available to local and regional entrepreneurs. Because there is typically such a long period between product invention to revenue generation in the technology sector, it is essential for technology businesses to obtain funding to sustain their operations until revenue generation occurs. We will play an important role in helping local and regional firms obtain the necessary investment and grant funding for new product development and company growth. For example, we will help identify equity capital sources by participating actively in two regional investor groups, the Alliance of Angels (as an honorary member) and the Delta Angel Group (as a sponsor), and in
other groups, as appropriate. We will continue to host seminars and other events to teach local entrepreneurs how to seek equity and federal R&D capital. By offering the Small Business Innovation Research/Small Business Technology Transfer (SBIR/STTR) Alerting Service and the Northwest Technology Investor Network, we will help entrepreneurs connect with funding sources. Likewise, we will help local entrepreneurs identify executive, technical, and advisory candidates through the Technology Job Connection service.

Strength in Numbers

We will lead an effort to identify and attract R&D operations of large corporations to locate near PNNL. A big factor in developing a thriving technology sector in the Tri-Cities is the need for more than just one large R&D organization (PNNL) here. Therefore, we are undertaking an effort to attract other large technology-based organizations to the local area. The first step, currently under way, is to identify the characteristics of PNNL that make it attractive as a neighbor to other technology-based organizations. In later steps, a subcontractor will identify industries and large firms that would benefit from having a facility near PNNL, and the Tri-City Industrial Development Council will be provided with a list of specific candidates to contact. We will work with other local organizations to make its property and technological resources available to desirable neighbors of PNNL.

The Source for Technology Business Information

We will create and provide information to enhance economic development outcomes locally and regionally. Our position as a national laboratory and connections with technology business advocacy organizations regionally give us unique access to information that helps foster technology-based entrepreneurism. We will continue to host educational seminars for entrepreneurs and provide the web-based Northwest Technology Investor Network, the SBIR/STTR Alerting Service, the monthly Tri-Cities Tech Business Update newsletter, the database “Organizations that Provide Support to Small Businesses and Entrepreneurs in Benton and Franklin Counties,” the Technology Job Connection website, and invited articles for regional science, business, and media publications, including a monthly column on local economic development in the Tri-City Herald. These information tools will help entrepreneurs find money, business opportunities, experienced management team members, and other sources of expertise.

PNNL will use its technology assets and connections to help shift communities into a tech-based economy that is significantly less dependent on Hanford funding. (See Appendix A for descriptions of partner relationships.)
7.2.3 Workforce Development Through University Collaboration and Science and Engineering Education

Our focus on workforce development programs for students, professional development of teachers/faculty, and science education reform in schools will increase the likelihood of a diverse and sufficient supply of stellar scientists and engineers for DOE, PNNL, and the nation/region.

Major Educational Outreach Programs

To support the education, diversity, and research objectives of DOE’s Office of Science (SC), PNNL, and our education partners, our wide range of programs, partnerships, and outreach efforts will span the pipeline from grade school to graduate school. We currently participate in all four SC education programs for undergraduate students, which include the Community College Institute, Pre-Service Teacher Fellowships, Science Undergraduate Laboratory Internships, and the Faculty and Student Teams program. By leveraging the funding supplied by SC, we will continue to expand the number of students impacted by these programs, with a goal of maintaining greater than 100 student participants per year in those SC programs.

Beginning in FY 2005, we will fully participate in the Laboratory Science Teacher Professional Development Program, the newest national education initiative of DOE’s Office of Workforce Development for Teachers and Scientists, designed to support the “teacher quality” provisions of the U.S. government’s No Child Left Behind legislation. If this program is fully implemented by DOE, we will host 75 to 100 teachers in various workshops and research experiences in FY 2005.

Using a strategic hire made in FY 2003 and the opportunity offered through the formation of the Office of Fellowship Programs, we will pursue external funding for student and professional development programs to augment our traditional base of support from DOE and PNNL. In FY 2004, we will submit a proposal to the National Science Foundation for a Research Experience for Teachers grant focused on community college faculty. Additional strategy areas designed to increase the number of students and teachers impacted by our outreach, reform efforts, and research programs, are described below.

Strategies for Increased Impact

We will be recognized nationally and regionally as playing a key leadership role in efforts to catalyze widespread improvements in science education, through the Washington State Leadership and Assistance for Science Education Reform Project. This program will expand to involve approximately 120 school districts and 440,000 students and teachers by 2005. Funding from the state and external sources will reach more than $5 million by 2005.

Our strategies will allow PNNL to fully participate in DOE’s national effort to encourage students from underrepresented groups to pursue scientific and technical careers. Historically, drawing underrepresented students from outside the region to the Pacific Northwest has proven very difficult. We will design and
complete a survey of our diverse student appointees to learn what their key decision-making points were in selecting our site. This survey will be implemented in FY 2004 and will guide new recruitment efforts. At the same time, we will enhance this initiative by focusing our efforts on successfully transitioning participants in our local precollege diversity programs into our postsecondary programs.

We will continue to provide internships for undergraduates, graduates, and postgraduates that create a pool of applicants for regular staff employment at PNNL. Laboratory-sponsored programs include teacher development programs, high school internships, undergraduate and graduate fellowships, and limited-term employment for postgraduates. To assess the efficacy of our education programs in leading to a valuable pool of applicants for regular staff positions, we will work with Human Resources to add a survey to the sign-on or orientation process that will track how many of our new hires had national laboratory education appointments, and what the value was. This will be implemented by FY 2005. The results will allow us to determine which kinds of experiences students find most valuable in the longer term.

Finally, we will continue to provide key education functions/services and processes that support a wide variety of university/Laboratory collaborations. Our University Relations program will house Master Agreements with those institutions we work with most often, while other focused agreements will be housed in individual groups or directorates. Each year, our University Relations program will assess all the Master Agreements to ensure that they continue to support the strategic needs of the Laboratory. Examples of our research and education collaborations are in the programmatic descriptions contained in this plan, and are described fully in Appendix A.

Of the research staff at PNNL, approximately 20 percent report having had an educational appointment at a national laboratory prior to becoming staff here. Of those, the vast majority indicated the experience was very important to their career decision.

Working with her mentor, Liyu Li, Creighton University student Kayli Hall examines the catalyst process that produces hydrogen from water using visible light. The Office of Basic Energy Sciences (BES) co-funds Kayli’s summer internship.

“My summer research has taught me that persistence, perseverance, and a questioning mind are the keys to being a good scientist. I hope to put the skills and knowledge that I have gained into use throughout my career.”

- Kayli Hall, intern
7.3 PNNL's Facility Strategy Delivers Enabling Infrastructure

PNNL has a facility strategy and the demonstrated ability to implement that strategy, which will provide world-class scientific user facilities for the nation’s science enterprise, core research facilities to support DOE programs, and partnership facilities that expand the regional science and technology base.

Strategy Overview

To accommodate our envisioned support to DOE programs, we have updated our strategy to aggressively reshape the PNNL campus with new user facilities, multiclient-funded core research facilities, and alternative-funded partner facilities. This strategy will allow rapid progress toward creating PNNL’s research campus of the future while reducing the Laboratory’s overall facility footprint and supporting the cost-effective cleanup of the 300 Area. To accomplish this, we will build upon our historical success in using innovative funding mechanisms and partnerships to acquire facility capacity. Module 7.3.1 provides details on our “Consolidated Laboratory” approach. In addition, we will focus on new scientific facilities where we can provide unique value. In summary, our facility strategy has three parts: maintain, divest, and move to new federally and alternatively funded buildings.

With our existing user facilities, we offer scientific researchers from across the globe access to state-of-the-art research capabilities. During this planning period, we maintain the relevancy of our existing user facility, and complement and extend our capability by proposing two new user facilities (see Module 2.0). Upon DOE initiating the facility acquisition process, we will submit a proposal to develop, deliver, and operate one of the four planned DOE Genomics:GTL facilities (see Module 2.6). Preliminary estimates place the building at 150,000 to 250,000 gross square feet (GSF), with a total estimated project cost of $175 to $225 million. Facility site selection is anticipated for FY 2004 along with the start of conceptual design. We are also developing a proposal for a DOE BES national complex interfacial catalysis user laboratory (see Module 3.7).

While PNNL user facilities act as an access portal to our capabilities, our core R&D facilities are the means by which our staff create and rapidly translate scientific discoveries into solutions for DOE programs. A significant portion of our core research capabilities are located in DOE-owned 300 Area buildings. Most of these facilities were built as part of the Hanford Site Cold War mission. Over the years, we have transitioned out of more than 100 obsolete facilities, but we still remain in 29 major buildings, many of which are contaminated or approaching the end of their useful life. As part of its overall responsibility for the Hanford Site, DOE is seeking to shorten the schedule and decrease the cost of the 300 Area cleanup (estimated at $300 million for PNNL facilities alone). The PNNL facility strategy proposes to consolidate its core research capabilities housed in 300 Area buildings.
The physical consolidation of PNNL’s modernized research campus into a single location will enhance the Laboratory’s ability to work in integrated teams.

Our Partnering Strategy

When DOE established PNNL, it expressed the expectation that PNNL use its vast scientific and engineering talent to expand the regions’ S&T capability, diversify and grow the local economy, and establish close and effective relationships with universities in the region, including joint participation in research activities. One means used by PNNL to achieve these ends is by entering into formal partnerships to acquire jointly shared research capabilities. In 2002, PNNL and WSU planned a joint science and engineering facility—the Bioproducts, Sciences, and Engineering Laboratory—as part of a collective research effort in bioproducts and related sciences research. The proposed 60,000 to 70,000 GSF multipurpose facility is sited on the campus of WSU, Tri-Cities, approximately one mile south of the main campus of PNNL. Facility construction by the State of Washington is scheduled to be completed by 2006. The facility will contain classrooms, laboratories, and offices for faculty and graduate students. It will also contain research laboratories that will be leased by PNNL. This arrangement will provide PNNL an opportunity to interact directly with university faculty and students and contribute to the development of regional scientific and engineering base. See Module 3.1.3.1 for details.

Other partnership activities to be pursued during this planning period includes exploring a teaming opportunity among our Marine Sciences Laboratory and universities in Washington State. The Marine Sciences Laboratory’s geographical location, technical expertise, and facilities present a clear opportunity to leverage these potential regional partners to address coastal and homeland security issues while creating educational and economical opportunities. More detail can be found in Modules 4.4 and 5.7.
7.3.1 PNNL’s Proven Approach to Provide State-of-the-Art Facilities

Our proven Consolidated Laboratory approach creates the means to provide state-of-the-art facilities while managing cost and risk.

In 1963, the government contract to operate Hanford Site research and development laboratories established the “Consolidated Laboratory,” essentially the first use of alternative financing concepts in the DOE Complex. It allowed the combined set of government and Battelle facilities and equipment, including a single workforce and set of management systems, to be used to operate the Laboratory as a single business enterprise for both maintenance and operations (M&O) activities and Battelle private work. In the 1980s, DOE and Battelle again employed the “Consolidated Laboratory” concept to obtain third-party funding for office and computer laboratory facilities to support programmatic needs. Utilizing commercial leases, five new buildings were authorized and constructed, each within approximately 18 months (total 340,000 square feet [sq ft]).

These five buildings will be core facilities capabilities sited next to EMSL. By lengthening lease and cancellation terms, specifying the conditions under which a lease can be canceled or transferred to a successor M&O contractor, and gaining Battelle ownership of the building at the end of 25 years, a substantial cost savings can be realized (within the parameters of acceptable risk). That savings is estimated at $1 million in the first year alone, growing substantially each year to total over $200 million over the next 40 years. During this planning, lease restructuring will be pursued to lower costs and risk to DOE. The five buildings include:

1. Information Sciences Building 1—a 50,000-sq-ft single-story office building housing 200 staff, providing a centralized location for PNNL’s Information Technology staff and the sub-network for the Atmospheric Radiation Measurement program.

2. Information Sciences Building 2—a 61,000-sq-ft single-story office and computer laboratory building with partial basement housing 250 staff and PNNL’s high-speed computing infrastructure and local area network servers.

3. National Security Building—a 100,000-sq-ft two-story office building with partial basement housing 400 staff and work spaces designed for classified and sensitive data.

4. Environmental Technology Building—a 100,000-sq-ft two-story office building with partial basement housing 355 staff and computational laboratory capabilities.

5. User Housing Facility—a two-story, 82-room guest house providing onsite accommodations predominately for EMSL users.
We are proposing, under the “Consolidated Laboratory” approach, to supplement federal facilities investments during the next five years with additional partnership and leased buildings. Proposed acquisitions include the Washington State University Bioproducts, Sciences, and Engineering Laboratory, which will provide office and laboratory space in partnership with the local university; and a state or privately financed office/laboratory building, which will provide office, research laboratory, and computational space in support of federally funded laboratory buildings.
7.3.2 Timing of 300 Area Cleanup Presents Opportunity and Risk to Our Research Campus of the Future Strategy

Although the 300 Area accelerated cleanup provides opportunity for a synergistic approach that reduces cleanup costs and enables the Laboratory to cost-effectively revitalize its infrastructure, it introduces the risk of interrupted research operations if new facilities are not constructed in time for a smooth transition.

The Office of Science (SC) has recognized the need to revitalize the aging infrastructure at its national laboratories. At the same time, the DOE Office of Environmental Management (EM), which is responsible for the ultimate decontamination and decommissioning of Hanford Site facilities, is working to accelerate this activity to reduce costs. For PNNL, this creates the opportunity for a synergistic approach that reduces cleanup costs and enables us to cost effectively revitalize our infrastructure. This is an opportunity to consolidate and co-locate core Laboratory capabilities that would benefit from shared infrastructure. This provides the added advantage of bringing together disciplines in an integrated fashion, enabling new scientific discoveries, and more rapid translation of these discoveries into deployable technological solutions.

Today, 3800 PNNL staff members conduct and support research activities on a campus composed of 79 buildings with nearly 2 million square feet. Approximately one-third of that space (about 700,000 sq ft) is located in the Hanford Site 300 Area. Most of the facilities in the 300 Area were built during the 1940s and 1950s to support fuel fabrication and testing for the nation’s defense production mission. Though the main 29 facilities PNNL occupies have been maintained and modernized, their basic configurations and locations reflect mission requirements of long ago. Many of the buildings, their utility distribution systems, and the ground they are sited on are contaminated. The average age of these buildings is 43 years and they have an estimated decontamination and decommissioning cost of $300 million. Additional information on building use, condition, and deferred maintenance can be found in Appendix B.

The 300 Area facilities that we operate represent:

- 60 percent of our general purpose laboratories
- 32 percent of our wet chemistry laboratories
- 55 percent of our filtered ventilation laboratories
- 100 percent of our hot cells
- 33 percent of our biology laboratories
- 100 percent of our fresh-water aquatic laboratories
- office space for about 800 staff members.

We are proposing a strategy that allows us to exit 300 Area facilities in a manner that enables us to complete ongoing programmatic activities and transition critical capabilities to new buildings outside the cleanup zone. We will consolidate our core
capabilities in radiological research, as well as a significant portion of advanced analytical chemistry, physical sensing, microbial biology, materials chemistry, and dosimetry capabilities into a smaller set of facilities located closer to the core Richland campus. The uncertainty of the accelerated cleanup schedule and the unknown effect of early cleanup activities on the operations of the buildings we occupy drive us to transition out of the 300 Area as soon as possible. Authorization of FY 2006 federal funding for new research facilities (see Module 7.3.3) is essential to our strategy.

To ensure that research capabilities and ongoing programs are available to support DOE missions, we will work with the DOE Richland Operations Office and the River Corridor cleanup contractor to identify a schedule that mutually supports accelerated 300 Area cleanup and the orderly transition of core research capabilities. We are pursuing alternative financing for a portion of the replacement buildings to augment requested federal facility funding. Where possible, we are disposing of legacy waste, reducing material inventories, and readying the buildings we occupy for transfer to the River Corridor cleanup contractor. We continue to invest in our core and user facilities outside of the cleanup zone to ensure their relevancy, readiness, and reliability. Though little opportunity exists, we are also relocating small portions of our capabilities to existing Battelle private buildings and available lease property.

To maintain uninterrupted support to DOE and DHS missions, PNNL and DOE must ensure that the accelerated Hanford Site cleanup schedule is integrated with PNNL’s campus modernization plan.

New core facilities will house capabilities that address critical national priorities.

(a) As part of the EM and SC organizational restructuring, a Pacific Northwest Site Office (PNSO) was established on December 5, 2003, to provide continued oversight of PNNL, which is currently being supported by EM’s Richland Operations Office through FY 2004.
7.3.3 The Next Five Years

During this planning period, PNNL will take actions to ensure that it has the facility capability required to meet its customer needs and achieve the Laboratory vision.

We understand the challenges presented in maintaining and modernizing the facilities that support our capabilities and the ramifications to the nation’s science programs if we are not successful. To ensure that we have the resources to add, upgrade, and maintain needed laboratories and infrastructure, the following key actions will be accomplished during the planning period:

- New user facilities/laboratories will be proposed that complement PNNL and EMSL capabilities.
- Lower long-term operating costs and risk will be achieved. One possible means is the restructuring of existing commercial leases.
- In partnership with WSU, we will complete construction of the shared Bioproducts, Sciences, and Engineering Laboratory in FY 2006. The design will be initiated during FY 2004.
- We will provide mission justification for funding of FY 2006 efforts to consolidate core research capabilities located in aged Hanford Site buildings into a smaller, new complex north of PNNL’s main campus. This multiclient funded space, estimated at a total of 300,000 to 350,000 square feet, is planned for FY 2009 construction completion. Approximately 70,000 square feet will be alternatively financed.
- Initially, we will propose to the Office of Science (SC), a new facility that will replace a portion of the capabilities currently located in the 300 Area. The 300 Area actions have provided an avenue to replace aged facilities with state-of-the-art facilities that will take the Laboratory into the future. This facility will allow PNNL to continue to build on its core capabilities in molecular, chemical, and environmental science. The facility will provide signature capabilities that bring new value to our current and future programs, such as systems biology and biotechnology, interfacial chemical catalysis, productive and efficient use of high-end computers, and information analytics. The proposed facility is anticipated to be approximately 90,000 to 110,000 gross square feet, and total estimated cost will be $60 million.
- We will also propose to the Department of Homeland Security (DHS), a new facility that will replace capabilities currently located in the 300 Area. The proposed building will provide a unique array of research in support of the mission capabilities for PNNL. The facility will focus on providing multipurpose laboratories that simulate various end-user applications, supporting R&D, cross-training, and tool validation (e.g., watch and warn, regional fusion centers, emergency response). It will also provide education and training areas and an industry/university/Laboratory collaborative environment without loss of security or privacy. The proposed facility is anticipated to be approximately 80,000 to 100,000 gross square feet, and the total estimated cost will be $55 million.
We will accelerate the 300 Area cleanup schedule and increase costs savings by readying facilities now occupied by PNNL for transfer to River Corridor cleanup contractor. Capabilities not core to PNNL future missions will be divested. During 2003, two PNNL buildings were vacated (332 and 3718S) and readied for decontamination and decommissioning by EM. Another building (6652E) was transferred to another government agency. Two additional buildings (3720 and 306W) will be vacated in FY 2004 and readied for decontamination and decommissioning. In parallel, legacy waste from the RPL will be processed and material inventories reduced as much as possible in preparation of transfer to the Hanford Site cleanup contractor.

We will maintain a level of maintenance and renewal investment in existing buildings that reflect building life-cycle considerations, ensure operational reliability, and enable transformational science. With the exception of EMSL, we will limit maintenance investments in Hanford Site DOE facilities to essential building systems and reconfigurations necessary to meet critical mission objections. This will result in a planned increase in deferred maintenance and deterioration in building conditions. Our FY 2005 Integrated Facility and Infrastructure crosscut budget reports an average maintenance investment without recapitalization of 1.5 percent for the planning period. Our facility strategy will in the short term drive this percentage down. Battelle will continue to adequately fund the life-cycle and modernization costs of its private buildings in which DOE work is performed. When possible, we will use IGPP funds for business or new capability development that enhance the Laboratory’s research capability and investments aimed at operational savings.

Our strategy reduces our existing deferred maintenance backlog by 94 percent ($34 million to $2 million) and consolidates our DOE facility footprint by approximately 150,000 gross square feet, replacing 40- to 50-year-old buildings with new modern facilities. By the end of the planning period, our success in implementing the facility strategy will contribute to the resolution of the Hanford Site legacy and create DOE’s enduring asset of regional S&T excellence. (see the proposed construction project table, Appendix B).

<table>
<thead>
<tr>
<th>Location</th>
<th>Area (Sq Ft) Millions</th>
<th>Area (Sq Meters) Millions</th>
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</thead>
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<td>DOE Main Site (300 Area)</td>
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<tr>
<td>DOE Leased</td>
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<td>0.007</td>
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<tr>
<td>Battelle Main Site (RCHN)</td>
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<tr>
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<tr>
<td>Battelle Leased</td>
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<tr>
<td><strong>Total</strong></td>
<td><strong>2.018</strong></td>
<td><strong>0.188</strong></td>
</tr>
</tbody>
</table>

PNNL partnerships with other government and private sector entities have doubled the facility square footage available to address DOE missions.
7.3.4 User Facilities Portal to PNNL

Through existing and proposed user facilities, the scientific community accesses PNNL facilities, equipment, and vibrant scientific community.

We offer scientific researchers worldwide access to state-of-the-art facilities, equipment, and research capabilities through our user facilities. For example, EMSL presents users with a comprehensive collection of unique and cutting-edge resources enabling solutions to problems in the environmental molecular sciences. Those resources are grouped into six primary facilities that focus on a broad spectrum of scientific issues. In addition, our atmospheric research Gulfstream-1 aircraft is a user facility available to both federal and private industry research. It is equipped with state-of-the-art atmospheric chemistry and physics instrumentation. Finally, we partnered with local government agencies to create Applied Process Engineering Laboratory, a user facility focused on transforming the output of fundamental science to applied solutions and economic development.

During this planning period, we are proposing two new user facilities. Upon DOE initiating a facility acquisition process, we will submit a proposal to develop, deliver, and operate one of the four planned DOE Genomics:GTL facilities. Our proposal will focus on our demonstrated capability in high-throughput mass spectrometry, imaging, systems biology, and operation of national user facilities. Module 2.6 discusses in detail PNNL’s role in this program. We propose to site the new user facility close to EMSL. The size of the building is initially estimated at 125,000 to 175,000 sq ft, with a total estimated project cost of $175 million to $225 million. Facility site selection is anticipated for FY 2004 along with the start of conceptual design. In support, PNNL and Battelle are currently investing in critical scientific proteomic programs and capabilities; thus, two systems biology prototype facilities are being established. The first is the prototype proteomics sample processing facility located in the LSL-2 Building and EMSL, and made possible through a combination of PNNL discretionary resources and Battelle capital investments. The other is the Microbial Cell Dynamics Facility located in the DOE-owned 331 Building.

To enable the U.S. scientific community to meet the challenge of the precise control of molecular processes by using catalysts, we are in the preliminary stages of developing a proposal for a BES national user facility for complex interfacial catalysis. The Complex Interfacial Catalysis Facility will provide the tools needed to advance catalysis science by enabling the development of the fundamental principles underlying catalytic phenomena and serve as a focal point of intellectual capital in the catalysis community. Additional programmatic detail is provided in Module 3.7. This proposal is in the very early stages, but the initial estimate places the facility at around 110,000 sq ft at a cost of $170 million.
One of the major attractions of a national user facility is its collection of state-of-the-art research capabilities housed in one location. To maintain the relevancy of our user facilities, investments in general building maintenance, building renewal, and next-generation scientific equipment capability are critical. Given the priorities for facility capital investments during this planning period, solutions for EMSL space needs will be limited to PNNL's existing footprint. The original design of EMSL allows for additional 36,000-sq-ft laboratory and 18,000-sq-ft office pods on the north end of the building. The possibility of a 27,000-sq-ft office/computer laboratory expansion located on the south end of the building that could add seminar and workshop capability has been examined. We anticipate that programmatic growth and user requirements will drive the need for these additions in the out-years.
Appendix A
Partnerships
Appendix A: Partnerships

University Partnerships and Collaborations

Partnerships between the U.S. Department of Energy’s (DOE’s) national laboratories and universities strengthen our nation’s intellectual and economic competitiveness. We are engaged in collaborative research and education initiatives with scientists at a wide variety of colleges and universities, both in the United States, and worldwide. Collaborative interactions with scientists and students at universities generate enthusiasm and new ideas through the sharing of insights, resources, and information. These interactions range from individuals from each institution participating in joint research sometimes supported by more formal arrangements such as Joint Research Institutes to support for teaching programs at regional colleges and universities. These collaborations in a diverse array of scientific and engineering disciplines serve to strengthen our capabilities, promote scientific discovery, provide educational opportunities, and bring together the best talent to work on DOE’s most challenging issues. The following are examples of important research collaborations with universities that support our Laboratory agenda, DOE missions, and other government agencies.

Bio-Based Processing

We take part in Collaborative Institute for Bioprocesses Research with Washington State University, University of Idaho, and the Idaho National Engineering and Environmental Laboratory (INEEL), and other universities.

Carbon Management and Climate Studies

We are a primary participant in the nation’s two largest research and development consortia focusing on terrestrial carbon sequestration: 1) Consortium for agriculture; Soils Mitigation of Greenhouse Gases with multiple midwest and western universities, and 2) Carbon Sequestration in Terrestrial Ecosystems Research and Development Consortium with Oak Ridge National Laboratory and multiple universities across the United States.

To characterize the geology of the Ohio River Valley, we collaborate with Battelle Columbus, British Petroleum (BP), American Electric Power, Ohio State University, and West Virginia University.

With the University of Alaska at Fairbanks and BP, we collaborate on use of carbon dioxide to produce methane from methane-bearing formations in aluminum.

As part of the Joint Global Climate Change Institute with the University of Maryland (U of M), we conduct multidisciplinary research in three primary areas related to scientific and policy study of global energy and the environment: 1) leading the development of integrated assessment approaches to climate change, 2) establishment of energy-efficiency centers and creation of nontraditional funding mechanisms for energy projects, and 3) understanding both the effect of climate changes and the associated social vulnerabilities these effects may create. Through the U of M relationships with the National Aeronautics and Space Administration and the National Oceanic and Atmospheric Administration, joint research efforts are strengthened.

More than 20 other universities partner with us in the Atmospheric Radiation Measurement Program to address some of the great uncertainties about greenhouse gases and the potential impact on global climate.
Appendix A—Partnerships

**Computer and Network Infrastructure Security**
We collaborate with the University of Idaho on computer hardware, network infrastructure security improvements, software to detect and deter intruders and preserve information integrity, and quality and security improvements of electronically mediated interactions.

**Computational Sciences**
Our Environmental Molecular Sciences Laboratory staff are active in collaborations in theory, modeling, and simulation with scientists from about 80 universities in the United States, and about 60 universities representing 60 countries.

**Environment and Health**
We are involved with the Superfund Basic Research Center with Oregon State University and Oregon Health & Science University to explore the effects of the nervous systems of environmental pollutants that contaminate water supplies.

We take part in Evergreen College's Student-Oriented Software program to explore distributed computing technologies to improve modeling systems in the Laboratory's Distributed Hydrology Soils Vegetation model.

We are involved in water resources research collaborations with regional universities to improve tools and understanding for better management of Pacific Northwest water resource management.

**Imaging Science and Technology**
We develop new methods for enabling humans to visualize and interact with three-dimensional datasets, in collaboration with the University of Washington.

We develop flexible architecture for integrating multiple image analysis stools with Pennsylvania State University.

Utah State University and Central Washington University each have image analysis collaborations with us that are planned and under way.

**International Security and Nonproliferation**
We are part of the Institutes for Global and Regional Security Studies with the University of Washington's Jackson School of International Studies and Department of Political Science and our Pacific Northwest Center for Global Security.

In addition, Princeton University, the University of California at Los Angeles, the University of Idaho, and Washington State University each have collaborations with PNNL that are important to technologies for nuclear arms control, nonproliferation, and verification activities vital to national security.

**Life Sciences**
Our Cell Systems Institute partnership agreement with University of Washington’s School of Medicine focuses on joint research coupling theoretical and experimental studies of cell-signaling components of the dynamic information control systems in cells.

The Massachusetts Institute of Technology, the University of California at San Diego, and the University of Utah each have other systems biology collaborative research with us under way.
The University of Arizona, Harvard University, the University of Texas at Austin, the University of Washington, and the Fred Hutchinson Cancer Research Center have continuing biology-related collaborative efforts with us.

**Nanoscience and Nanotechnology**

Our Joint Institute for Nanoscience with the University of Washington focuses on particles films and nanoclusters for a variety of applications. This partnership is also supported by the National Science Foundation to support creation of new course work and incorporating distance learning tools in various nanoscience and nanotechnology areas.

Our Microproducts Breakthrough Center is a collaborative effort with Oregon State University to develop and help to market advances in microtechnology in our region.

**Nuclear Energy**

The University of Texas’s Nuclear Engineering School is our partner in the DOE Nuclear Energy Research Initiative proposal to study and develop shielding materials for advanced light water reactor pressure vessels. With the University of California at Berkeley, we partner to develop an advanced nuclear fuel. With the University of Michigan, we conduct joint research materials for current and advanced nuclear reactors. The University of Illinois partners with us to evaluate basic mechanisms of interfacial deformation of materials. We collaborate with regional universities to promote the entry of students into the professions related to nuclear energy science and research.

**Remote Sensing Applications**

The Northwest Energy Technology Collaborative partners us with INEEL, the University of Washington, Idaho State University, Oregon State University, and the University of Idaho to improve the delivery of remote sensing and related spatial information technologies and applications from developer to end users.

**Waste Characterization and Management**

With several universities, we collaborate to solve waste disposal problems at the Hanford Site. Partnerships are active with Washington State University and Yale University to develop strategies for treating tank wastes. Washington State University analyzes material composition of tank wastes using laser ablation and mass spectrometry. With the University of Idaho, we partner on water sequestration and sonic methods for detecting plugs in waste transfer pipelines. Oxidation pathways in organic ion exchange media is our collaboration with Texas Tech University, and the University of California at Santa Barbara is our partner in materials separation research.

Our Natural and Accelerated Bioremediation Research Program with Washington State University and Montana State University is a collaboration in stopping movement of toxic metals in groundwater and soils at DOE facilities. We partner with New Mexico State University, Florida State University, Oregon Health & Science University, Oregon State University, and the University of Michigan to research other waste management areas. Our research under a DOE Environmental Management Science Program, with Oregon State University examines interactions between microbiological and hydrological processes in the unsaturated zone.
Instrumentation and Students
We partner with Heritage College to provide guidance and other support regarding the development of a horticultural initiative in the cultivation and propagation of native plants. We also provide adjunct faculty support to the teaching programs in environmental science and computer science. Students and faculty from Heritage College benefit from internships and research appointments at the Laboratory.

Oregon Universities System
A Memorandum of Understanding among the multiple universities in the Oregon University System with the Laboratory forms a cooperative relationship for research and educational activities, collaborations in the life, physical sciences, and economic development.

Northwest Virtual Entrepreneurial Support Network
Partners at PNNL and the Oregon Technology Transfer Council comprise the technology transfer officers from Oregon’s research universities.

Washington State Universities, Tri-Cities
A collaborative program in systems biology is the newest of the regular and graduate courses at the local branch campus. PNNL staff members also teach short courses at the Washington State University Professional and Continuing Education Program.

The Consolidated Information Center (CIC) is our Hanford Technical library collection with the Washington State University library. The DOE Public Reading Room is also located at the CIC and operated by PNNL. The CIC also provides space for a Life Sciences Laboratory, museum, and conference rooms that are available to DOE and its contractors.

Industrial Partnerships and Collaborations

The DOE Office of Science’s Laboratory Technology Research Program supports a number of partnership projects with private industry to bring together the best talent and address DOE’s most challenging issues. These cost-shared projects help to translate basic research advances to commercial applications over a broad spectrum of scientific disciplines such as advanced materials science, intelligent chemical processing, efficient manufacturing, sustainable environmental technology, and innovative biotechnology. We also work with and support local and regional businesses through technical assistance programs that help to diversify the local economy and create new jobs. Types of support to small businesses include resolving technical problems, testing and evaluating products and materials, and improving manufacturing processes.
Our industrial partnerships may also involve a broad variety of public and private institutions. In our science mission, we participate with DOE, other national laboratories and federal agencies, private companies, universities, and foreign research institutes in the Atmospheric Radiation Measurement Program to improve general circulation models used in climate research and to resolve scientific questions about greenhouse gases and their impact on global climate.

We participate in the Natural and Accelerated Bioremediation Research Program, a DOE Office of Biological and Environmental Research fundamental science research program on subsurface biological systems and their application to bioremediation, whose participants include DOE multiprogram national laboratories, several universities, and industrial participants.

In our environmental quality mission, we participate actively in the Environmental Management Science Program focusing Laboratory projects under this program on managing tank wastes and in situ treatment of groundwater. We partner with several industrial organizations on projects where the work directly supports critical DOE science needs for cleanup. We teamed with the Project Hanford management contractor, Fluor Hanford, to manage technology development for Hanford Site cleanup activities and to provide innovative solutions to expedite cleanup activities at the Plutonium Finishing Plant.

In our national security mission, we bring together the resources and highly specialized expertise needed to address the multidisciplinary nature of many national security issues, such as counterterrorism, weapons nonproliferation, and information security. We participate in the International Nuclear Safety Program, with the objective of reducing the risks of operating Soviet-designed nuclear reactors by working cooperatively with host countries of the former Soviet Union on nuclear safety and supporting technical infrastructure.

The Foundation for Russian American Economic Cooperation is a strategic Laboratory partner, which dates to the origins of the Nuclear Cities Initiative. We served as a key partner in establishing the International Development Centers in two of Russia's closed nuclear cities. Since this initial collaboration, the Foundation has continued to serve in this capacity under direct contract to DOE.

As part of the National Bureau of Asian Research, we have entered into a strategic alliance under the auspices of the Laboratory's Pacific Northwest Center for Global Security. We will provide science and technology knowledge and expertise in support of a new initiative titled Tracking the Strategic Environment in Asia. The program will track significant developments from Central Asia and Russia through south, northeast, and southeast Asia and across the Pacific to the United States. Under our sponsorship, the National Bureau of Asian Research received a grant from DOE's National Nuclear Security Administration to provide strategic analysis of the Asian security environment.

Partnerships in our energy resources mission address the difficult technical issues facing energy providers and consumers and provide industrial involvement from basic research through development, to ensure direct deployment of the results in industry.
We participate in the Solid-State Energy Conversion Alliance, which brings together Laboratory and industrial capabilities in material sciences, chemical processing, sensors, and modeling to develop and mass-produce clean, affordable, and high-efficiency modular solid-state fuel cell technology for diverse power needs in multiple market areas. We are working with the Washington Technology Center, Bonneville Power Administration, and other northwest organizations to implement the vision for a Northwest Regional Energy Collaborative. We have a partnership with Celerity and 6th Dimension for the EnergyWeb Project with Bonneville Power Administration. We will participate in the Massachusetts Institute of Technology's Consortium on Protocols for Dynamic Energy Control. We will assist Utility Automation Integrators, Inc., in the design and enhancements of the Dispatch 2.0 product, select a site for implementation of the outage management system demonstration in Alabama, and deploy an operational system at the site.

In the **building industry**, we work to advance and advocate the energy-efficient and environmentally sound design and construction of the nation's buildings. Our efforts include working with industry consensus standards organizations, such as the American Society of Heating, Refrigerating and Air Conditioning Engineers, and national model energy code organizations, such as the International Code Council, to develop progressive building energy codes and standards. We assist the states in the adoption/upgrade, implementation, and compliance processes by developing and distributing code compliance tools, materials, and services, and have provided approximately 40 states with individualized technical assistance. Our Emerging Technologies Program involves coordination with appliance and lighting manufacturers, and supports DOE's goal of advancing the development and sales of highly efficient new and emerging technologies.

In the **automobile industry**, we play a major role in the Northwest Alliance for Transportation Technologies, which addresses national technological challenges by focusing relevant industrial and research capabilities on specific transportation goals such as lightweight materials and emission controls. This partnership combines the strengths of national laboratories, research universities, and industrial manufacturers. The DOE Office of Transportation Technology supports this highly innovative, cost-sharing partnership with PACCAR (Bellevue, Washington, maker of Kenworth and Peterbilt trucks) and Freightliner (Portland, Oregon), the leading producers of heavy trucks in the United States. The partnership also supports active programs with the engine manufacturers to reduce diesel emissions in cost-shared partnership with Caterpillar, Ford, General Motors, DaimlerChrysler, and Cummins Diesel. These programs also support DOE's transportation focus in government industry partnerships in FreedomCAR and 21st Century Truck.

In the **electronics industry**, we focus on semiconductor materials science. We work with Oak Ridge National Laboratory and Motorola on development of new high-k dielectric films on silicon materials. We are working with eV Products, Inc., of Saxonburg, Pennsylvania, and Washington State University on a project to improve the availability of cadmium zinc telluride crystals.
In the agricultural industry, we partner with grower groups and processors in the corn industry, the National Corn Grower's Association, the Iowa Corn Promotion Board, and Archer Daniels Midland in a joint effort to create new nonfood markets for agricultural products as renewable alternatives to petroleum. A regional Collaborative Institute for Bioproducts Research is being formed by our Laboratory, INEEL, Washington State University, and the University of Idaho that will develop technologies for renewable biomaterials, such as potato waste and wheat bran, for chemical manufacturing.

In support of the nuclear power industry, we are working toward partnerships with leading developers of next-generation nuclear power plants where we can contribute expertise to diagnostic and prognostic instrumentation and controls, radiation materials sciences, fuel technologies, and waste processing. We participate in the Shelter Implementation Program Project Management Unit, which is a joint venture of Bechtel Corporation, Battelle, and Electricite de France to manage the European Bank for Reconstruction and Development program to stabilize the remains of the Chornobyl Unit 4 reactor. We plan to partner with nuclear engineering companies that are developing the next generation of modular nuclear reactors.
Appendix B
Pacific Northwest National Laboratory
Key Facilities
Appendix B: Pacific Northwest National Laboratory Key Facilities

2400 Stevens Building

The 2400 Stevens Building occupies 93,000 square feet (sq ft) and is located at 2400 Stevens Drive in Richland. PNNL has been an occupant of this facility since 1979. It is a general research facility and contains multiple types of space including laboratories and offices. The structure consists of a two-story office section and high bay laboratories. All of the laboratories are on the first floor, and are classified as light chemistry or electronic.

Pacific Northwest National Laboratory (PNNL) occupies the entire building, which is considered a core research facility for PNNL. Work conducted at 2400 Stevens contributes to DOE’s four mission areas, with most of the research activities focused on energy security.

Applied Process Engineering Laboratory (APEL)

Process Science and Engineering Complex

APEL is located at 350 Hills Street in Richland. The 90,000-sq-ft building is a joint community project sponsored by the Port of Benton, the City of Richland, and DOE through PNNL. APEL serves as an incubator facility that any company, agency, or individual can use to test the commercial potential for new business concepts and innovative technologies. The facility is designed to foster interaction and collaboration between the various occupant groups. Three PNNL technical groups occupy 26,000 sq ft of laboratory and office space.

APEL offers a single-story office wing, two floors of laboratories, and a 28-foot high bay. The existing structure, built in 1975, was modified to meet APEL needs beginning in 1997 and was dedicated in March 1998. Battelle has a lease in APEL for the space PNNL occupies in the building. Most of PNNL’s work at APEL is focused on environmental research, including vitrification technologies. The facility provides linked government/private facilities for research and chemical process studies.

Chemical Sciences Laboratory (329 Building)

The 329 Building is a DOE-owned facility located in the Hanford Site’s 300 Area. The two-story facility, built in 1952, has a partial basement and offers 39,000 sq ft of space. The building was substantially updated in 1994. The interior consists of standard laboratories, maintenance shop, offices, and counting rooms with one-foot-thick concrete walls and ceilings. Numerous “caves” constructed of lead bricks have been built to work with radioactive materials. The Neutron Multiplier Facility was added in 1974.

Battelle/PNNL has had sole operational responsibility for the 329 Building since 1987. Research conducted in the facility supports all four DOE mission areas, but the vast majority of the work is national security related.
William R. Wiley Environmental Molecular Sciences Laboratory (EMSL)

EMSL, a 200,000-sq-ft DOE-owned national user facility, opened in 1997 and is the newest building at PNNL. EMSL is located at 3335 Q Avenue, in the heart of PNNL’s main research campus. The two-story building houses advanced scientific instrumentation and computing resources, dry and wet laboratories, a state-of-the-art auditorium, office space, and conference rooms.

Hundreds of scientists from around the world travel to EMSL annually to conduct research in the facility's collaborative environment; others take advantage of EMSL's unique electronic capabilities to pursue projects from offsite locations via the Internet. Although research conducted at EMSL supports all of DOE's mission areas, most of the facility's work is focused in basic science disciplines.

Life Sciences Laboratory-1 (331 Building)

The 331 Building is located in the south end of Hanford's 300 Area, adjacent to the Columbia River. The 115,000-sq-ft facility, owned by DOE, is a three-story, reinforced concrete building with laboratories on the first and third floors and a mechanical service floor between them. In addition to administrative offices that were part of the initial structure built in 1970, office space was added during modifications in 1982 and 1996.

The nature of the work activities conducted in the 331 Building is largely composed of biological and chemical studies directed at impacts on living organisms, both surface and subsurface. The building is equipped with many unique features to facilitate this research, including aquatic laboratories and accredited animal care facilities. Radioactive materials are also permitted within the building in accordance with prescribed limitations.

Marine Sciences Laboratory (MSL)

The MSL, located in Sequim, Washington, is owned by Battelle. Primary buildings at the MSL consist of MSL1, a beach laboratory of 13,000 sq ft established in 1963, and MSL5, the “Uplands Facility” established in 1982 and containing 24,000 sq ft. MSL1 is a wood-frame facility made up of two wet laboratories with the capability to support research with seawater organisms. MSL5 is also a wood-frame building with offices, a conference room, and 10 laboratories, including one configured to handle radionuclides.

MSL was established to provide capabilities for advancing and applying state-of-the-art technology, techniques, and knowledge in the marine and aquatic sciences to address emerging needs in management of marine and estuarine systems, national security research, evaluation of the effects of human activity on such systems, and development of marine resources and biotechnology. A third building at MSL, MSLTRL1, is a Battelle-leased 3,300-sq-ft modular structure that provides critical office space at the beach facility.
Material Science Laboratory (326 Building)

Located in Hanford's 300 Area, the DOE-owned 326 Building was constructed in 1953. The 63,000-sq-ft building features offices, wet and dry laboratories, and a concrete basement. Operational responsibility was assigned to Battelle in 1989. The primary mission of the two-story facility is analysis of metallurgical samples of post-irradiated materials (reactor components, fuel elements, and construction materials to evaluate characteristics and performance).

The metallurgical mission continues within the building, as well as the other missions: the development of radioactive materials detectors, the analysis of air filter samples routinely removed from all PNNL radioactive materials laboratories, and support for the other nonradioactive laboratories like EMSL. The building has the capability to do radiological work. Although the facility's research connects with all DOE mission areas, the majority of the work performed here is national security oriented.

Math Building

The Math Building was built in 1967 and is owned by Battelle. Located at 906 Battelle Boulevard in the main PNNL research campus, it is a single-story building of almost 30,000 sq ft. The facility was designed and originally used as a support office that contained two large computer laboratories. These mainframe computers were used for computational processes to support research and business operations. It is a designated research laboratory because of its LAN, high-speed computing infrastructure, and connection to the EMSL at PNNL.

Currently the building is largely used to provide additional user space during peak EMSL workloads. Most of the work conducted in the Math Building supports DOE's fundamental science mission.

Physical Sciences Laboratory (PSL)

The PSL is a two-story research laboratory located at 908 Battelle Boulevard in the main PNNL research campus. This Battelle-owned building was constructed in 1967 and contains more than 90,000 sq ft. The first floor of the building is primarily nonradiation wet chemistry physical sciences laboratories and adjacent office space. The basement area contains wet and dry laboratories with adjacent offices, six shop areas, and mechanical rooms. There is also a special room designed especially for the storage of hazardous materials. PSL research supports all four DOE mission areas.

Radiochemical Processing Laboratory (325 Building or RPL)

The 325 Building, owned by DOE, is located in Hanford's 300 Area. It was built in 1953, contains nearly 145,000 sq ft, and has historically provided support to the environmental management cleanup mission at the Hanford Site. The 325 Building
continues to support work on other environmental and fundamental science projects, providing an important link to PNNL’s molecular science capability and is uniquely equipped to manage work involving unsealed radioactive source terms.

The building is constructed on three levels and contains a mixture of laboratory and office space, as well as operating system workspaces. The building is designated as Hazard Category II nuclear building and, as such, has undergone the strictest form of Battelle’s Integrated Operations Management process.

Research Operations Building (ROB)

The ROB is located at 902 Battelle Boulevard in the main PNNL research campus. Built in 1969 and owned by Battelle, the ROB serves as the central corporate office building at PNNL. In addition to executive offices, ROB houses key PNNL functional organizations, such as Strategic Planning, Auditing, Communications, Finance, Facilities and Operations, and Human Resources. The building, nearly 70,000 sq ft in size, contains two floors.

Research Technology Laboratory (RTL)

Located at 520 Third Street in Richland, the RTL is owned by Battelle, which bought the 56,000-sq-ft facility from Douglas Aircraft in 1982. RTL’s main building, RTL 520, contains wet chemistry laboratories, dry laboratories, and adjacent administrative offices. It is one of only two facilities in the North Richland area in which radiological work can be performed. Assorted other storage, warehouse, and shop buildings make up the RTL complex.

National Security Building (NSB)

The NSB is predominantly an office building housing a significant portion of PNNL’s National Security Directorate staff. The two-story building, located at 3230 Q Avenue in the main PNNL research campus, offers 100,000 sq ft and is a Battelle-leased facility. It contains Limited Area Island workspaces, which allow for work involving classified and sensitive data. NSB also houses the Office of the Associate Manager for Science and Technology for the DOE Richland Operations Office\(^{(a)}\), which has oversight responsibility for PNNL.

Information Sciences Buildings 1 and 2 (ISB1 and ISB2)

These mirror-image buildings were constructed in 1991 at the north end of the main PNNL research campus and are Battelle-leased facilities. ISB1 (50,000 sq ft) is located at 3350 Q Avenue; ISB2 at 3320 Q Avenue. Both are predominantly office buildings, providing centralized locations for PNNL’s Information Technology staff. ISB1 contains the sub-network for the ARM project, which is a fundamental science project with dependency on information technology resources. ISB2 (60,000 sq ft) houses PNNL’s high-speed computing infrastructure and LAN servers.

\(^{(a)}\) As part of the EM and SC organizational restructuring, a Pacific Northwest Site Office (PNSO) was established on December 5, 2003, to provide continued oversight of PNNL, which is currently being supported by EM’s Richland Operations Office through FY 2004.
Analytical and Nuclear Research Laboratory
(320 Building)

The 320 Building is located in Hanford’s 300 Area. Built in 1965, the nearly 31,000-sq-ft facility is a DOE-owned building. The current missions include radiochemical environmental analyses, sample preparation, methods development, and classified programs using analytical procedures.

Special instrumentation available in the 320 Building includes various mass spectrometers, electron-beam microscopes, x-ray diffraction, and radiation counters.

In addition to limited office space, the first floor of the facility contains wet type chemistry laboratories, a portion of which are operated as clean rooms and are supplied with high-efficiency particulate air (HEPA)-filtered supply air. The remainder of the main floor laboratories are wet-type chemistry laboratories supplied with filtered exhaust air. The basement consists of primarily electronic type laboratories, a filter room, and a mechanical room.

Biological Sciences Laboratories

The Biological Sciences Laboratories include the Microbial Cell Dynamics Laboratory Cellular Observatory, high-field mass spectroscopy, high-field nuclear magnetic resonance, and Molecular Science Computing Facility (all part of EMSL), all which support biological, proteomic, microbial, and ecological research.

Gulfstream Aircraft and Atmospheric Radiation Monitoring Sites

Gulfstream Aircraft and Atmospheric Radiation Monitoring Sites are unique user facilities for atmospheric monitoring.
Appendix B—Pacific Northwest National Laboratory Key Facilities

Required Facilities and Infrastructure Tables and Charts

<table>
<thead>
<tr>
<th></th>
<th>DOE Office of Science Facilities</th>
<th>Other DOE Facilities</th>
<th>All DOE</th>
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<tbody>
<tr>
<td></td>
<td>Total</td>
<td>Active</td>
<td>Non Operational Excess</td>
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<tr>
<td>Number of Facilities</td>
<td>29</td>
<td>23</td>
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<tr>
<td>Square Footage (SF in millions)</td>
<td>0.7</td>
<td>0.7</td>
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<tr>
<td>Deferred Maintenance ($ in millions)</td>
<td>26</td>
<td>26</td>
<td>8</td>
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<tr>
<td>Replacement Plant Value ($ in millions)</td>
<td>300</td>
<td>300</td>
<td>101</td>
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<tr>
<td>Deferred Maintenance Condition Index</td>
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Deferred Maintenance and Replacement Plant Value by Program Secretarial Office

Deferred Maintenance Condition Index by Use Code

Active Facility Age Profile by Use Code

Use and Condition of Active DOE Owned Laboratory Space
Overall Condition of DOE Owned Space

<table>
<thead>
<tr>
<th>Active Facility</th>
<th>Replacement Cost in Current Dollars</th>
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<tbody>
<tr>
<td>DOE Owned Total</td>
<td>401 Million</td>
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<tr>
<td>Battelle Owned Total</td>
<td>99 Million</td>
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Active Facilities Replacement Values

<table>
<thead>
<tr>
<th>Major Construction Projects</th>
<th>TEC</th>
<th>2003</th>
<th>2004</th>
<th>2005</th>
<th>2006</th>
<th>2007</th>
<th>2008</th>
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<tr>
<td>Proposed Construction</td>
<td></td>
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<tr>
<td>Program Line Items Projects</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>DOE Genomics:GTL Whole Proteome Analysis Facility (BER)</td>
<td>175</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>60</td>
<td>70</td>
<td></td>
</tr>
<tr>
<td>WMD Proliferation Prevention (NNSA/ DHS)</td>
<td>55</td>
<td>1</td>
<td>5</td>
<td>20</td>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>GPF Line Items Projects (SLI)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Multipurpose CPBR Science Building</td>
<td>60</td>
<td>1</td>
<td>6</td>
<td>20</td>
<td>20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TOTAL PROPOSED CONSTRUCTION</td>
<td>290</td>
<td>-</td>
<td>1</td>
<td>7</td>
<td>31</td>
<td>100</td>
<td>105</td>
</tr>
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</table>
Appendix C
Pacific Northwest National Laboratory Profile
September 2003
Appendix C: Pacific Northwest National Laboratory Profile, September 2003

Pacific Northwest National Laboratory (PNNL) is a U.S. Department of Energy (DOE) multiprogram national laboratory that creates new knowledge and delivers solutions to science and technology challenges across DOE’s science, national security, environmental quality, and energy resources missions. The Laboratory is an outgrowth of the research and development (R&D) component of the Manhattan Project Hanford Works that focused on materials science, nuclear technology, and health studies. Strengths in chemical science and engineering, materials science and engineering, biological science and technology, computational science and information technology, nuclear science and engineering, environmental sciences and engineering, and engineering of integrated systems underpin our research programs. We operate the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility with advanced resources for fundamental research on physical, chemical, and biological processes. Our biological science research focuses on the biomolecular basis of health effects from environmental pollutants. We solve legacy environmental problems with cost-effective cleanup solutions and technologies that prevent pollution and minimize waste. Our scientists identify technology to characterize and mitigate the consequences of pollution, climate change, and other environmental impacts. We develop clean energy and industrial processes, lightweight materials and advanced power systems for transportation, and efficient building technologies for DOE’s energy mission. We provide impactful and innovative solutions to prevent the proliferation of weapons of mass destruction, combat terrorism, promote nuclear safety, and protect critical infrastructure and information for DOE’s national security mission. The Laboratory strives for excellence in management and safe operations, thereby enabling efficient and cost-effective research while protecting our workers, the public, and the environment. Our staff members are broadly engaged in local economic development, education, and other community activities.

Distinctive Competencies and Major Facilities

PNNL operates 183,000 square meters (1,982,000 square feet) of facilities, most of which are located in Richland, Washington. The centerpiece of our research facilities is the EMSL with its state-of-the-art research equipment, including a new high-performance supercomputer (11.8 Tflop) and a 900-MHz, high-field nuclear magnetic resonance spectrometer, as well as mass spectrometry and surface science instruments. Our Biological Sciences Laboratories support biological, toxicological, proteomic, microbial, and ecological research. The Radiochemical Processing Laboratory provides innovative processes for environmental cleanup and beneficial uses of radioactive materials, including facilities for nuclear fuel chemistry and waste characterization. The Process Science and

<table>
<thead>
<tr>
<th>Laboratory Information</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Location:</strong> Richland, Washington</td>
</tr>
<tr>
<td><strong>Number of Full-Time Equivalent Employees:</strong> 3,868 (as of September 2003)</td>
</tr>
<tr>
<td><strong>Scientific and Technical Degrees:</strong> 706 PhD; 556 MS; 629 BS</td>
</tr>
<tr>
<td><strong>Contractor:</strong> Battelle</td>
</tr>
<tr>
<td><strong>Accountable Program Office:</strong> Science</td>
</tr>
<tr>
<td><strong>Field Office:</strong> Richland Operations Office(a)</td>
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<td><strong>Web Site:</strong> <a href="http://www.pnl.gov">http://www.pnl.gov</a></td>
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<tr>
<td><strong>Science:</strong> $104.9 million</td>
</tr>
<tr>
<td><strong>Nuclear Energy:</strong> $1.7 million</td>
</tr>
<tr>
<td><strong>Energy Efficiency and Renewable Energy:</strong> $33.0 million</td>
</tr>
<tr>
<td><strong>Environmental Management:</strong> $53.6 million</td>
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<tr>
<td><strong>Nonproliferation and National Security:</strong> $155.9 million</td>
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<tr>
<td><strong>Other DOE:</strong> $23.0 million</td>
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<tr>
<td><strong>Non-DOE:</strong> $179.6 million</td>
</tr>
<tr>
<td><strong>Total Funding:</strong> $561.0 million</td>
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(Note: Budget data are for FY 2003 and exclude remediation funds.)

(a) As part of the EM and SC organizational restructuring, a Pacific Northwest Site Office (PNSO) was established on December 5, 2003, to provide continued oversight of PNNL, which is currently being supported by EM’s Richland Operations Office through FY 2004.
Engineering Complex and the Applied Process Engineering Laboratory provide linked government and private-user facilities for thermal energy and chemical process studies. Our research-equipped Gulfstream aircraft and our role as manager of the Atmospheric Radiation Monitoring (ARM) Program provide unique user facilities for atmospheric monitoring. We also operate the Marine Sciences Laboratory in Sequim, Washington, for oceanic and estuarine ecosystem research as well as coastal security. Our distinctive capabilities (described below) underpin the Laboratory's research programs.

- **Chemical Science and Engineering.** Trace and complex analyses, including instrument design; molecular modeling, including structures; radiochemistry; interfacial catalysis and advanced separations; micro chemical and thermal systems; chemical and biochemical process design and control.

- **Material Science and Engineering.** Macro- and nano-scale synthesis; materials manufacturing; environmental and radiation degradation; glass and high-temperature oxide (fuel cell) performance.

- **Biological Science and Technology.** Microbial systems; analyses and modeling of biomolecules and biomolecular systems; biological effects of radiation and chemicals; dosimetry.

- **Computational Science and Information Technology.** Large-scale data management; problem-solving environments; high-performance computing in molecular sciences; computer system design and security; information analytics and visualization.

- **Nuclear Science and Engineering.** Trace detection and analysis; reactor safety; fuel-cycle processes and related security systems; nuclear-based detectors; non-destructive evaluation.

- **Environmental Sciences and Engineering.** Atmospheric measurement and remote sensing; climate modeling; geo- and biogeochemistry; fate and transport of contaminants; ecological monitoring, management, and remediation; integrated assessments and policy.

- **Engineering of Integrated Systems.** Device and system design and control; diagnostics and prognostics; robotics; systems engineering and assessments; integrated security systems; energy codes and standards.

## Key R&D Activities

**Science and Technology Mission.** The Laboratory provides the scientific tools and knowledge to support DOE mission needs in biology, atmospheric science and global environmental change, materials and chemical sciences, national security, and computational science. Major research activities include:

- Study of the mechanism of cellular responses to insults; research focus areas include proteomics, cell imaging, computational biology, mass spectrometry, and nuclear magnetic resonance spectrometry.

- Development of innovative science-based technologies for chemical, biological and nuclear detection.

- Study of complex coupled biological and geochemical processes that control the fate and transport of environmental contaminants and their remediation of contaminated areas by biological processes.
Research into the fate and effects of energy-related emissions in the atmosphere, modeling of climate processes and the potential effects of climate change on key natural resources and human activities, and air quality and the coupling between meteorology and chemistry.

Experimental, theoretical, and computational study of structures and processes of molecular and nanoscale systems catalysis, energy storage, sensors, and subsurface contaminant migration, synthesis and chemical physics of oxide materials, single-molecule spectroscopy and high-resolution biological imaging, advanced electronic structure methods, reaction rate theories, and accurate interaction potentials for molecular simulations.

Study of molecular interactions at interfaces, growth of hierarchically ordered materials, self-assembly methods in materials synthesis, metallurgy and ceramics, and mechanical property studies carried out under substance hostile chemical or physical environments.

Development of high-performance computing environments by intimately coupling hardware, software, advanced algorithms, and domain-specific methods to address extraordinarily complex problems, for applications in chemistry, biochemistry and biophysics, environmental science, nanoscience, computer science, and applied mathematics.

Environmental Quality Mission. Principal research focus areas include spent fuel materials and surface chemistry; tank waste treatment and vitrification; safety assessments; characterizing, containing, and treating subsurface contaminants; managing land and marine ecosystems; and social, economic, health, and policy assessments. Activities include:

- Development of technologies to treat and immobilize stored radioactive and hazardous wastes, and technologies to remove, immobilize, and destroy subsurface organic and metal contaminants using chemical, thermal, and biological means.
- Development and use of advanced techniques to monitor and characterize radioactive and chemical wastes, and contaminated soils and groundwater systems.
- Development of tools and approaches for managing and restoring natural resources, assessing ecosystem health and impacts from possible land uses, and integrating the economic, social, and political factors that influence land-use decisions.
- Studies of marine chemistry, ecological processes, resources, animal and plant health, and adaptive ecosystem management, with emphasis on characterizing sources, fates, and effects of chemical contaminants.
- Measurement of exposures to radioactive and chemical agents, and development and use of analytical tools to assess and predict human health impacts.
- Technical, social, and economic studies supporting life-cycle management and formulation of sound environmental policies and regulations.
- Development and use of geohydrological models and data for predicting the performance of remediation technologies and waste disposal sites.

National Security Mission. Research supports the U.S. national security objectives to detect, monitor, prevent, and reverse the global proliferation of weapons of mass
destruction, protect the U.S. homeland, and support transformation of the military for modern mission requirements. We develop, demonstrate, and deploy technologies and systems that support the monitoring of treaties and agreements; detect and analyze physical and chemical signatures of weapons of mass destruction; design, develop, and demonstrate tritium production in light-water reactors and tritium-extraction technology; and conduct research relative to care and protection of humans in combat situations, enhanced information analysis and visualization for decision support, protection of critical elements of the national energy and communications infrastructure, and enhancement of law enforcement and anti-terrorism. Activities include:

- Development and deployment of new analytical, statistical, and computational methods, and information analysis technologies to help identify and communicate potential threats to the U.S. homeland.
- Partnering with academic, nongovernmental, and international organizations to address traditional and nontraditional issues related to global security and non-proliferation.
- Training international and U.S. border enforcement officials to thwart the smuggling of chemical, biological, or nuclear materials across foreign borders.
- Development and use of ultrasensitive nuclear radiation detection and analysis systems to monitor creation and control of nuclear materials.
- Development of integrated systems for detecting, characterizing, and decontaminating biological warfare pathogens and chemical agents.
- Development of strategies for threat vulnerability assessment, risk management, emergency response, information assurance, and infrastructure protection.
- Design and demonstration of in-reactor assemblies and separations processes to produce tritium for national defense.
- Development of new sensors, data fusion, and non-destructive inspection technologies for extending the life of aging military systems and infrastructure.
- Providing technical support to U.S. and Russian surplus plutonium disposition activities through development of immobilization and "burning" technologies.
- Development and implementation of technologies and policy support to improve the safety of nuclear power generation and disposal of nuclear material in countries of the former Soviet Union.
- Development and use of advanced materials and sensors for improved collection, separation, and detection of nuclear, chemical, and biological material.
- Lead international cooperative science and technology programs that develop and apply state-of-the-art technologies and systems to promote nuclear safety and address issues of international security and regional stability.

Energy Resources Mission. Principal research focus areas support secure, clean, and affordable energy including advanced material and component designs for high-efficiency cars and heavy trucks; high-efficiency and low-cost modular solid-oxide fuel cells, standards and technologies for energy-efficient buildings; technologies for clean, productive, and sustainable industries of the future; and distributed power generation and electrical storage systems. Activities include:
- Development of advanced surface analytical facilities to characterize advanced catalyst surface for reduced clean-burn engine exhaust.
- Design of lightweight materials (particularly metal alloys), and development of design and manufacturing techniques for high-efficiency vehicle components.
- Development of engineered materials and system designs for fuel cells, batteries, and capacitors for transportation and distributed power generation.
- Creation and use of computational engineering and virtual prototyping to support component design, processing, and advanced life-cycle manufacturing.
- Development of advanced communications and controls to enable a transformational change in electric service and the use of distributed energy solution.
- Development and deployment of new technologies, controls, and energy standards to improve the energy efficiency of homes and buildings.
- Development of new technologies in advanced nuclear power systems and information sciences that will meet anticipated energy needs within increasingly stringent economic and environmental constraints.
- Development of new technologies to improve industrial processes and reduce both material requirements and process byproducts in the forest product, glass, chemical, and agricultural industries, and improving the processes for the sequestration and capture of CO$_2$.
- Development of new catalyst formulations, and understanding and application of new fungal strains in new production processes, enabling conversion of biomass materials to commercially available products.

Key Accomplishments

Nanosciences and Technology (1998 to present). We developed methods to synthesize nanoscale matter and integrate it into macroscale devices, thereby creating new functional materials from the bottom up. We developed tailored molecular assemblies to produce self-assembled monolayers on mesoporous oxide support materials for special applications in chemical separations, microelectronic circuits, photocatalysis, waste management, and sensing. We created arrays of nanoparticles with anomalously high stability and photocatalytic properties. We demonstrated that arrays of oxide nanowires display fundamentally different catalytic activity compared to their bulk materials. In electronics, we developed dilute magnetic semiconductor films that retain strong magnetization above room temperature, enabling experiments on spin-dependent charge conduction and spin injection across interfaces.

Systems Biology and Proteomics (1998 to present). To study signaling networks in cells, we developed sophisticated tools in proteomics, microbial dynamics, the cellular observatory, and biological modeling. For example, our state-of-the-art capabilities in high-throughput proteomics allow rapid identification of large amounts of protein complexes simultaneously, and successfully measure the expression levels of all proteins of the bacteria Deinococcus radiodurans in a single experiment. Identifying the proteins that allow this microorganism to survive in high-radiation environments could provide important insights to radiation biology and lead to novel approaches to waste cleanup. We are applying capabilities to support the DE Genomics/GTL Program and develop a new class of environmental biomarkers. The National Institutes of Health established PNNL as a base for proteomics research worldwide with a five-year, $10.2-million grant to foster scientific collaboration on important biomedical projects and to advance the understanding of the way human cells function.
Global Climate Assessment (1989 to present). We helped establish and continue to lead DOE's ARM Program, which focuses on understanding the role of clouds and atmospheric aerosols in climate change, providing scientists data to better understand and model climate dynamics. We developed specialized regional climate models to study the potential local impacts of climate change. We demonstrated that a warmer climate in the Pacific Northwest could have a drastic impact on the snow pack in the near coastal mountains, affecting both energy resources and agricultural activity. We are the world leader in integrated assessment models for understanding the dynamics of technology choice, economics, and environmental impacts on a global scale. Our work demonstrated the importance of shifting attention from emissions reduction to stabilizing the concentrations of greenhouse gases in the atmosphere. PNNL and its collaborators developed a state-of-the-art geographic information-based model for examining large-scale U.S. deployment of carbon capture and sequestration technologies.

Computational Sciences (1989 to present). The Laboratory developed a new generation of research tools for high-performance computing on massively parallel computers to address previously intractable scientific problems in computational chemistry, reactive transport in the subsurface and the atmosphere, and biological process simulations ranging from proteins to cells to organs. The Molecular Science Software Suite (MS3) extends the size and scale of chemical and biochemical problems that can be accurately studied. The developers of MS3 received a 1999 R&D-100 Award and a 2000 FLC Technology Transfer Award. We developed the highly successful SPIRE software for visual information mining for intelligence analysis, law enforcement, public health, patent analysis, and logistics. SPIRE also received a 1996 R&D-100 Award. We have also led advances in supercomputing ranging from the 256-GGlop IBM SP 512 processor computer acquired in 1996 and 1997 to the new 11.8-Tflop massively parallel Linux Itanium-2 based cluster from Hewlett Packard.

Biogeochemistry (1988 to present). We developed expertise and capabilities to address scientific issues fundamental to understanding the biogeochemical factors and processes controlling the microbial reduction of iron, technetium, uranium, and other contaminants in the environment. Our research in subsurface science is advancing our molecular-level understanding of surface chemistry. We are a major contributor to DOE's Natural and Accelerated Bioremediation program, and our studies have provided important insights for DOE-site cleanup decisions.

Subsurface Science (1983 to present). Through our research in contaminant transport and fate in the subsurface environment, we developed computer models that incorporate biogeochemical and hydrogeologic processes, predict chemical species, and show how they move in the subsurface. We identified microorganisms in the deep subsurface that may aid in remediation methods, and the PNNL-developed In Situ Redox Manipulation, which won an R&D-100 Award in 1998, modulates the subsurface geochemistry to immobilize contaminants.

Arms Control and Nonproliferation (1970 to present). We demonstrated technical, policy, and program leadership in the development and deployment of innovative technologies for international arms control and non-proliferation imperatives, including interagency efforts to reduce the number of nuclear weapons and amounts of weapons-grade material both in the United States and the countries of the former Soviet Union. Our staff was instrumental in developing and achieving congressional approval for the concept of Debt for Nonproliferation (DfN), which
involved pardoning the debt of foreign nations in exchange for weapons reductions. We developed statistical techniques for analyzing seismic activity from weapons tests. We developed automated instruments (such as the R&D-100 Award-winning Radionuclide Aerosol Analyzer and the Automated Radioxenon Analyzer) and other sensitive nuclear detection technologies and systems that are used for monitoring treaty compliance, weapons proliferation, and illicit materials trafficking. We created safeguards and security programs for accountability and control of special nuclear material in the United States and abroad. Our work on information analysis, dismantlement of nuclear warheads, cleanup and accountability of nuclear materials in North Korea and the countries of the former Soviet Union, fissile materials disposition, and nuclear materials protection and accountability increased global security. We have contributed to the Nuclear Cities Initiative and the Initiative for Proliferation Prevention, which help the Russian Federation reduce the size of its nuclear weapons establishment, and redirect work of nuclear weapons scientists to non-weapons-based activities.

Homeland Security (1970 to present). Scientists and engineers at PNNL were helping secure our homeland long before the terrorist attacks of September 11, 2001. We assessed the vulnerability of critical infrastructures across the nation as well as teamed with organizations to ensure our air and seaports are protected from the threat of terrorist attacks. The Laboratory has trained international and U.S. border enforcement officials to thwart the smuggling of chemical, biological, or nuclear materials across borders, and has supported the Department of Homeland Security by providing leadership in the procurement and deployment of radiation detection systems at ports of entry around the United States. The Laboratory also is providing expertise to the International Atomic Energy Agency to help locate, identify, and secure orphan, or unprotected, radioactive materials to reduce the possibility they would be used in the manufacture of dirty bombs.

Energy Technologies (1970 to present). The Laboratory helped to develop energy-efficient building standards, metering equipment, and design tools such as MECcheck (winner of a 1997 FLC Award). Staff worked with industry groups and more than 20 states to deploy these tools and standards, which are projected to save U.S. consumers $2 billion annually in energy costs. We developed energy-equipment diagnostic technology and software, such as Decision Support for Operations and Maintenance (DSOM) (winner of a 2001 R&D-100 Award). We developed new microtechnologies to improve or replace mobile and distributed power systems. Through public-private partnerships, such as FreedomCAR and the 21st Century Truck Programs, the Laboratory developed lightweight materials, advanced emission technologies, and auxiliary power units for transportation that will meet fuel-efficiency and emission goals. We extended our materials chemistry and ceramic processing capabilities in solid oxide fuel cells to focus on fuel cell system design, modeling, and fabrication. We also provide leadership in the Consortium for Electric Reliability Technology Solutions and the development of advanced communication and controls technologies to benefit a highly connected electricity grid and distributed energy systems.

Waste Management and Environmental Technologies (1965 to present). The Laboratory has characterized and evaluated problems related to legacy nuclear and chemical wastes and contaminated sites. We developed options for high-level nuclear waste disposal, screened potential repository sites, developed advanced decontamination
and decommissioning technologies, and demonstrated the suitability of waste forms and treatment options, including vitrification. We led the national Tanks Focus Area Program to develop, test, and deploy technical solutions for remediating the radioactive tank wastes stored at DOE sites. We are developing technologies to solve DOE and industrial environmental problems, including new chemical separation methods to reduce waste volumes, techniques to manipulate the subsurface and destroy or contain contaminants, processes for treating and immobilizing high-level wastes, and advanced instrumentation for process inspection, monitoring, and control.

Radiation and Chemical Health Effects (1950 to present). PNNL and its predecessor laboratories at Hanford have conducted fundamental radionuclide toxicology and radiation biology studies in support of radiation protection standards. We developed new instruments, materials, calibration methods, and facilities for detecting and analyzing radiation and chemical agents. These tools protect workers, workplaces, and the environment. Recent accomplishments include broad application of the more sensitive optically stimulated luminescence dosimeters (R&D-100 Award winners in 1992 and 1999), and real-time dosimeters for the National Aeronautics and Space Administration's space shuttles. We also developed real-time "breathalyzer" monitors to measure worker exposures to hazardous chemicals and toxic agents.

Nuclear Science and Technology (1950 to present). PNNL and its predecessor laboratories at Hanford have contributed to civilian nuclear power system design, technical foundations for regulations, operator training and qualification, and reactor safety. Accomplishments include development of alternative reactor designs; development and commercialization of fuel design, fabrication, and reprocessing techniques; design support to the Fast Flux Test Facility; demonstrating tritium production in light-water reactors; and purification of derived isotopes for medical and industrial applications. The Laboratory was a major contributor to the first quantitative assessment of reactor accident risks, and to the resolution of critical materials and other technical issues affecting reactor safety and regulation. The Laboratory also supported DOE's health and environmental response to the Chornobyl accident, and is making significant contributions to improving the safety of the nuclear industry in the countries of the former Soviet Union.

Advanced Scientific Instruments (1950 to present). PNNL and its predecessor laboratories at Hanford have been involved in developing and testing advanced instruments for detection and analysis in support of scientific research. In recent years (1992 to present), we increased the sensitivity, precision, and analytical usefulness of mass spectrometers and associated hardware for protein identification and rapid detection of chemical and biological agents. Continued progress in nuclear magnetic resonance spectroscopy and microscopy provided new information on tissue composition and the functions and structures of complex biomolecules. We improved matrix-assisted laser desorption and ionization mass spectrometry for rapid detection of microorganisms, and we advanced high-performance, field-portable, electrospray ionization, Fourier transform ion cyclotron resonance instrumentation. Advanced scientific instruments have important applications in national security, health, and environmental research. These important new technologies resulted in several R&D-100 awards, Federal Laboratory Consortium awards, and commercial applications.
Major Partnerships and Cooperative R&D Agreements

Science and Technology Mission. In PNNL’s Science and Technology mission area, a wide range of academic partnerships have been established to promote both scientific discovery and education. Laboratory and industrial partnerships bring the best talent to address DOE’s most challenging problems, and the EMSL user facilities serve the broader scientific community. Descriptions of these partnerships follow.

- With its nearly 1000 users, EMSL serves as a center for collaborative scientific research for the national and international academic and industrial community. The facility houses state-of-the-art research instruments for studying surface and molecular chemistry, advanced molecular and cellular biology, and computational modeling and simulation.

- DOE national laboratories, including PNNL in the leadership position, and universities are participating in the ARM Program, a DOE global climate change research project that focuses on resolving scientific questions about greenhouse gases and their impact on global climate. Long-term field measurements are obtained to study the distribution of energy and water in earth’s climate system.

- As participants in the DOE Genomics:GTL Program, researchers from PNNL and Oak Ridge National Laboratory are teaming to develop novel technologies that examine live cells and isolate, identify, and characterize groups of protein complexes within microbial cells to help solve problems in energy production, environmental cleanup, and carbon cycling.

- Seven DOE laboratories, more than 15 universities, and two industrial partners are participating in the Natural and Accelerated Bioremediation Research Program, a DOE Office of Biological and Environmental Research fundamental science research program focused on subsurface biological systems and their potential application to bioremediation.

- Researchers from PNNL and the University of Washington are involved in two major partnerships: the Northwest Institute for Nanoscience and Technology and the Joint Program for Cell Signaling. The Northwest Institute for Nanoscience and Technology supports our Laboratory-level initiative in nanoscience and strengthens our capabilities in biomaterials and in surface science. The Joint Program for Cell Signaling focuses on developing tools, computational resources, and technologies for measuring and predicting changes in the interactions of molecules that comprise living cells.

- PNNL and the University of Maryland have teamed to establish the Joint Global Research Institute. The Joint Global Research Institute meets the needs of a diverse set of clients for policy-relevant research, integrating the social sciences and natural science aspects of global change. It brings diversity and integrated tools to address issues such as globalization, regional and local effects, time spans on the order of centuries, complex human and non-human systems, risk, efficiency, and uncertainty.

- PNNL also is involved in high-performance computing partnerships with four other DOE national laboratories (Argonne, Brookhaven, Lawrence Berkeley, and Oak Ridge National Laboratory), Cray Inc., Hewlett Packard Inc., and IBM.

Environmental Quality Mission. In the Laboratory’s Environmental Quality mission area, PNNL, industry, and university partnerships span the development life cycle from basic science to final deployment, and provide comprehensive solutions to
DOE's complex environmental problems and related problems facing industry. Descriptions of these partnerships follow.

- DOE national laboratories, universities, and industrial partners are participating as teams in DOE's Environmental Management Science Program. The focus of PNNL's projects under this program is managing tank wastes, in situ treatment of groundwater, and health effects. We partner with several organizations on projects where the work directly supports critical DOE science needs for cleanup.

- PNNL is working with DOE and its Hanford contractors to develop technologies to safely and efficiently remediate radioactive waste in storage tanks, stabilize and dismantle facilities used for weapons production, and protect the Columbia River from residual contaminants in groundwater and subsurface soil at the Hanford Site.

- PNNL has teamed with university and industrial groups to establish the Microproducts Breakthrough Institute, a research and educational collaboration dedicated to the emerging and highly promising field of microtechnology and to the rapid commercialization of new microtechnology applications.

National Security Mission. In PNNL's National Security mission area, partnerships bring together the Laboratory's broad science base and highly specialized expertise to address the multi-disciplinary nature of many national and global security issues, such as counter-terrorism, weapons nonproliferation, and information security. Descriptions of these partnerships follow.

- PNNL has teamed with other DOE laboratories, U.S. firms, and host countries to participate in the National Nuclear Security Administration's International Nuclear Safety Program. This program reduces risks of operating Soviet-designed nuclear reactors by working cooperatively with host countries of the former Soviet Union on nuclear safety issues and by supporting the technical infrastructure upgrades needed for safe operations.

- PNNL is teaming with other DOE laboratories, industry partners, and universities to establish two new centers to support DOE's National Security mission area: the National Visual Analytics Center and the ARDA Northwestern Regional Research Center. The National Visual Analytics Center will provide national expertise in coordinating Department of Homeland Security visual analysis needs, evaluating and deploying technologies, designing new technologies, and creating educational curricula for new academic programs. PNNL hosts the ARDA Northwestern Regional Research Center, which has been established to solve information technology "challenge problems" for the benefit of the U.S. intelligence community.

- PNNL, the University of Washington (the Henry M. Jackson School of International Studies), and other universities in the Northwest have established the Pacific Northwest Center for Global Security. This Seattle-based center links PNNL with northwest universities and nongovernmental organizations to provide a forum for addressing and solving traditional and nontraditional nonproliferation and security issues. Partnerships include the Joint Institute for Global and Regional Security Studies at the University of Washington. Through PNNL support, the University of Washington promotes teaching, research, publication, and public outreach on security issues of regional and global concern to the United States.
Energy Resources Mission. In PNNL’s Energy Resources mission area, partnerships provide essential information about the technical issues facing energy providers and energy consumers, and provide industrial involvement — from basic research through development — to ensure direct deployment of the results in industry. Descriptions of these partnerships follow.

- PNNL, other DOE laboratories, and industrial partners have teamed to create the Solid-State Energy Conversion Alliance. This partnership works to pool capabilities in materials science, chemical processing, sensors, and modeling to develop clean, affordable, and high-efficiency modular solid-state fuel cell technology.

- State and federal government, industrial partners, and DOE laboratories are teaming to establish national building standards and guidelines. PNNL chairs the largest energy-standard-setting committee for the American Society of Heating, Refrigerating, and Air-Conditioning Engineers.

- Several universities, DOE laboratories, and industrial partners have teamed with PNNL to create the Northwest Alliance for Transportation Technology and the Advanced Communications and Controls Program. The Northwest Alliance for Transportation Technology is a public/private partnership that addresses transportation technology goals. Its focus is on developing low-cost, lightweight materials, advanced emission technologies, and auxiliary power units to meet the goals of the FreedomCAR and the 21st Century Truck programs. The Advanced Communications and Controls Program will focus on development of specific distributed energy technologies, interconnection standards, and models for determining the distributed generation impacts on transmission systems.

- PNNL, Idaho National Engineering and Environmental Laboratory, the University of Idaho, and Washington State University are teaming to form a new Northwest Bioproducts Research Institute. This institute will focus on developing a multi-disciplinary R&D program that will examine and develop methods for converting agricultural and food-processing residues and wastes into bio-based fuels, power, and industrial products, such as chemicals for plastics, solvents, and fibers.

*Includes safeguards and security, Bonneville Power Administration, and funds in Cooperative Research and Development Agreements.
Appendix D
Resource Projections
Appendix D: Resource Projections

The charts and tables contained in this appendix show Pacific Northwest National Laboratory (PNNL) funding and full-time equivalent (FTE) levels for years 2002 through 2008. Summaries of this information, provided in Module 1.1.3, profile the levels of actual budget authority and FTEs for the past fiscal year, the current year’s projections based on formal notifications, and future expectations based on proposal and customer interaction.

Assumptions and Definitions

The following assumptions and definitions were used in preparing this information:

Table D.1—Funding by Secretarial Officer
- Department of Homeland Security is called out separately in the resource projection table and descriptions are found in the Mission Area Module 4.5 of this plan.
- Funding by the Department of Health and Human Services is called out separately, as required.
- Work for Others shows funding from the National Institutes of Health separately, as required.
- Each instance of Work for Others over $1 million is called out separately in resource projection tables. The following Work for Others plans are described in Mission Area modules in this plan:
  - U.S. Department of Defense—Module 4.6 and 4.6.1
  - U.S. Army Corp of Engineers (3T Other Federal Agencies)—Module 5.5
  - U.S. Nuclear Regulatory Commission—Module 3.6
  - U.S. Environmental Protection Agency—Module 5.5
  - U.S. DHHS/National Institutes of Health—Module 2.5

Table D.2—Direct Personnel by Secretarial Officer
- Department of Health and Human Services is called out separately.
- Work for Others shows funding from the National Institutes of Health separately.

Table D.3—Resources by Major DOE Areas
- DOE effort includes net of transfer to other DOE contractors.
- Does not include proposed construction line item funding for replacement general purpose facilities.

Table D.4—Work for Others
- Includes optimistic case resource projections.
Input to the DOE Work for Others Program Report

PNL’s Work for Others (WFO) programs are an important complement to its support to the DOE’s multiple missions.

We select and manage our WFO activities to maximize value to DOE, the sponsoring agencies, and the Laboratory. Specifically, we believe that WFO programs promote:

- help other governmental agencies by making unique national laboratory capabilities available to them to solve their most complex scientific challenges. By extension, our WFO programs do not include work that can be performed satisfactorily by private organizations.

- build staff and infrastructure capabilities and create new technologies that are then available to DOE missions in science, energy, national security, and environmental quality. These programs increase opportunities to transfer technologies to productive applications in the private sector.

- provide additional overhead resources that the Laboratory invests in improved facilities, new research equipment, and innovation of new ideas.

We manage our WFO programs in close collaboration with our DOE programs to ensure these mutual benefits. The FY 2004-2008 Institutional Plan reflects this close integration by including the descriptions of its WFO programs in the appropriate DOE mission chapters. We introduce the WFO programs in the Laboratory’s Strategic Plan (Chapter 1), to define their roles in the Laboratory’s overall strategy. Details on each of the WFO programs are then provided in discrete modules in the mission chapters. These WFO modules describe the current and future work, value to the sponsoring agencies, and the benefits to related DOE programs. We provide all of the required funding tables in an appendix. The significant WFO programs that we currently envision including are for the National Institutes of Health, Nuclear Regulatory Commission, Department of Defense, Environmental Protection Agency, National Aeronautics and Space Administration, and private firms. The level of detail provided on several of these programs has been reduced to accommodate the need for additional security around some information.

Safeguards and Security Program Funding and DOE-SC Restructure

During FY 2004 (and prior years) the majority of the Laboratory’s Safeguards and Security (SAS) Program was funded by DOE-EM and included as part of the Hanford Site’s SAS program (direct) funding. The funding model for this support activity assumes “flat” funding is received each year. However, the Laboratory’s work involving national security assets continues to grow. If SAS funding remains “direct” for FY 2005, oversight and funding responsibilities have been requested to be transferred from EM to SC. A letter to DOE Headquarters was submitted from the DOE Field Office outlining this transfer for FY 2005 and beyond. The infrastructure and planning is under way to accommodate this shift from EM to SC, as well as to establish the reporting channels (through SC).
PNNL’s current SAS budget (direct, with programmatic overhead [OH] adders) needing to be “absorbed” by the Laboratory OH is projected at ~$11,100 thousand (target - no protective force) less $1,222 thousand current WFO G&A OH funding. This excludes $1,360 thousand programmatic request over target for export control and cyber security enhancements. Just as the protective force budget (i.e., Hanford Patrol) was re-assigned to a Hanford contractor when it shifted from OH to direct, a return to overhead funding could be expected in the future (an additional $2,200 thousand). The Laboratory’s share of Benton County Sheriff Office (~$200 thousand unburdened), RL\(^{(a)}\) Security Clearances support (~$160 thousand), vulnerability analysis costs, and alarm monitoring may be returned to the Laboratory overhead budgets. All this is expected to increase the Laboratory G&A OH rate by about five points, and increase the demand for General Purpose Equipment capital.

\(^{(a)}\) As part of the EM and SC organizational restructuring, a Pacific Northwest Site Office (PNSO) was established on December 5, 2003, to provide continued oversight of PNNL, which is currently being supported by EM’s Richland Operations Office through FY 2004.
## D.1 Funding by Secretarial Officer

(Budget Authorization $ in Millions)

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**Assistant Secretary for Energy Efficiency and Renewable Energy**

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(a) U.S. Customs funding moved from WFO to DHS in FY 2004.
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| DHS Effort (Department of Homeland Security)   |      |      |      |      |      |      |      |
| Total Direct Personnel                         | -    | 74.6 | 91.3 | 96.0 | 97.8 | 99.9 | 30.2 |
## Institutional Plan FY 2004–2008

### Work for Others Effort (WFO)

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### Laboratory Direct

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### Total Laboratory Indirect

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### Total Laboratory Personnel (FTE)

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(a) U.S. Customs funding moved from WFO to DHS in FY 2004.
## D.3 Resources by Major DOE Areas

(Budget Authorization $ in Millions)

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| Direct Personnel             |      |      |      |      |      |      |      |
| Operating                    | 268  | 265  | 294  | 345  | 372  | 372  | 400  |
| Capital Equipment            | 7    | 2    | 20   | 34   | 34   | 47   | 49   |
| General Purpose Equipment — GPE | -    | 0    | 1    | 1    | 1    | 1    | 1    |
| General Plant Projects — GPP | 6    | 7    | 8    | 9    | 11   | 12   | 12   |
| Construction Line Item       | -    | -    | 1    | 6    | 24   | 71   | 83   |
| **Total Direct Personnel**   | 281  | 275  | 324  | 395  | 441  | 504  | 546  |

Assistant Secretary for Energy Efficiency and Renewable Energy

| Operating                    | 3.5  | 4.9  | 5.6  | 6.9  | 8.7  | 8.7  | 8.3  |
| Capital                      |      |      |      |      |      |      |      |
| General Purpose Equipment — GPE | -    | -    | -    | -    | -    | -    | -    |
| General Plant Projects — GPP | 6    | 7    | 8    | 9    | 11   | 12   | 12   |
| Construction Line Item       | -    | -    | 1    | 6    | 24   | 71   | 83   |
| **Total Operating**          | 26.9 | 31.1 | 32.9 | 40.0 | 40.5 | 53.0 | 55.9 |
| Capital                      |      |      |      |      |      |      |      |
| General Purpose Equipment — GPE | -    | -    | -    | -    | -    | -    | -    |
| General Plant Projects — GPP | 6    | 7    | 8    | 9    | 11   | 12   | 12   |
| Construction Line Item       | -    | -    | 1    | 6    | 24   | 71   | 83   |
| **Total Capital**            | 3.9  | 4.1  | 4.5  | 5.0  | 6.0  | 8.0  | 9.0  |
| **Total Funding**            | 26.9 | 33.0 | 32.9 | 40.0 | 40.5 | 53.0 | 55.9 |

Assistant Secretary for Fossil Energy

<p>| Operating                    | 6.4  | 7.6  | 7.6  | 8.6  | 9.6  | 11.1 | 12.1 |
| Capital                      |      |      |      |      |      |      |      |
| General Purpose Equipment — GPE | -    | -    | -    | -    | -    | -    | -    |
| General Plant Projects — GPP | 6    | 7    | 8    | 9    | 11   | 12   | 12   |
| Construction Line Item       | -    | -    | 1    | 6    | 24   | 71   | 83   |
| <strong>Total Operating</strong>          | 7.1  | 8.6  | 8.1  | 9.1  | 10.1 | 11.6 | 12.6 |
| Capital                      |      |      |      |      |      |      |      |
| General Purpose Equipment — GPE | -    | -    | -    | -    | -    | -    | -    |
| General Plant Projects — GPP | 6    | 7    | 8    | 9    | 11   | 12   | 12   |
| Construction Line Item       | -    | -    | 1    | 6    | 24   | 71   | 83   |
| <strong>Total Capital</strong>            | 0.3  | 0.4  | 0.4  | 0.4  | 0.4  | 0.4  | 0.4  |
| <strong>Total Funding</strong>            | 7.4  | 9.0  | 8.5  | 9.5  | 10.5 | 12.0 | 13.0 |</p>
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(a) U.S. Customs funding moved from WFO to DHS in FY 2004.
## Appendix D—Resource Projections

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<td>75.7</td>
<td>91.5</td>
<td>92.6</td>
<td>102.9</td>
<td>109.5</td>
<td>129.0</td>
<td>138.4</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>210</td>
<td>273</td>
<td>291</td>
<td>277</td>
<td>281</td>
<td>319</td>
<td>348</td>
</tr>
<tr>
<td><strong>Total Laboratory Funding</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Operating</td>
<td>517.1</td>
<td>584.3</td>
<td>575.0</td>
<td>589.8</td>
<td>610.9</td>
<td>646.8</td>
<td>561.7</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>1,395</td>
<td>1,415</td>
<td>1,397</td>
<td>1,366</td>
<td>1,385</td>
<td>1,396</td>
<td>1,407</td>
</tr>
<tr>
<td>Capital Equipment</td>
<td>9.1</td>
<td>7.3</td>
<td>5.7</td>
<td>6.4</td>
<td>6.6</td>
<td>6.9</td>
<td>7.0</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>8</td>
<td>4</td>
<td>22</td>
<td>36</td>
<td>36</td>
<td>49</td>
<td>51</td>
</tr>
<tr>
<td>General Purpose Equipment-GPE</td>
<td>0.1</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>General Plant Projects-GPP</td>
<td>3.9</td>
<td>3.8</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>8</td>
<td>7</td>
<td>8</td>
<td>9</td>
<td>11</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>Construction Line Item</td>
<td>0.9</td>
<td>-</td>
<td>1.0</td>
<td>5.0</td>
<td>20.0</td>
<td>60.0</td>
<td>70.0</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>-</td>
<td>-</td>
<td>1</td>
<td>6</td>
<td>24</td>
<td>71</td>
<td>83</td>
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<tr>
<td>Landlord Line Item</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Direct Personnel</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Indirect Personnel</td>
<td>1,376</td>
<td>1,395</td>
<td>1,411</td>
<td>1,420</td>
<td>1,425</td>
<td>1,429</td>
<td>1,433</td>
</tr>
<tr>
<td><strong>Gross Laboratory Funding</strong></td>
<td>531.0</td>
<td>596.4</td>
<td>586.1</td>
<td>605.7</td>
<td>642.0</td>
<td>718.2</td>
<td>643.2</td>
</tr>
<tr>
<td><strong>Total Personnel</strong></td>
<td>2,786</td>
<td>2,821</td>
<td>2,840</td>
<td>2,838</td>
<td>2,881</td>
<td>2,958</td>
<td>2,988</td>
</tr>
<tr>
<td>DOE Site Transfers and Cash Work</td>
<td>(63.1)</td>
<td>(40.4)</td>
<td>(41.1)</td>
<td>(10.5)</td>
<td>(10.2)</td>
<td>(9.7)</td>
<td>(9.6)</td>
</tr>
<tr>
<td><strong>Net Laboratory Funding</strong></td>
<td>467.9</td>
<td>559.9</td>
<td>545.1</td>
<td>595.2</td>
<td>631.7</td>
<td>708.5</td>
<td>633.6</td>
</tr>
</tbody>
</table>
D.4 Laboratory Funding Summary\(^{(a)}\)
(including optimistic case DHS project)

To properly set the FY 2004 Work for Others Ceiling, as required, this chart and table show the optimistic case for all WFO resource projections including the projected funding level from a DHS project.

<table>
<thead>
<tr>
<th>Year</th>
<th>2002</th>
<th>2003</th>
<th>2004</th>
<th>2005</th>
<th>2006</th>
<th>2007</th>
<th>2008</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Effort</td>
<td>441.4</td>
<td>409.0</td>
<td>361.1</td>
<td>371.6</td>
<td>371.3</td>
<td>384.3</td>
<td>385.0</td>
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<tr>
<td>DHS Effort</td>
<td>-</td>
<td>83.8</td>
<td>364.5</td>
<td>115.4</td>
<td>130.1</td>
<td>133.4</td>
<td>38.3</td>
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<tr>
<td>Work for Others</td>
<td>75.7</td>
<td>91.5</td>
<td>92.6</td>
<td>102.9</td>
<td>109.5</td>
<td>129.0</td>
<td>138.4</td>
</tr>
<tr>
<td><strong>Total Operating</strong></td>
<td><strong>517.1</strong></td>
<td><strong>584.3</strong></td>
<td><strong>826.2</strong></td>
<td><strong>589.8</strong></td>
<td><strong>610.9</strong></td>
<td><strong>646.8</strong></td>
<td><strong>561.7</strong></td>
</tr>
<tr>
<td>Capital Equipment</td>
<td>9.1</td>
<td>7.3</td>
<td>5.7</td>
<td>6.4</td>
<td>6.6</td>
<td>6.9</td>
<td>7.0</td>
</tr>
<tr>
<td>General Purpose Equipment-GPE</td>
<td>-</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>General Plant Projects-GPP</td>
<td>3.9</td>
<td>3.8</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td>Construction Line Item</td>
<td>0.9</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>10.0</td>
<td>55.0</td>
<td>68.0</td>
</tr>
<tr>
<td>Landlord Line Item</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Gross Laboratory 1830 Funding</strong></td>
<td><strong>531.0</strong></td>
<td><strong>596.4</strong></td>
<td><strong>836.4</strong></td>
<td><strong>600.7</strong></td>
<td><strong>632.0</strong></td>
<td><strong>713.2</strong></td>
<td><strong>641.2</strong></td>
</tr>
<tr>
<td>DOE Site Transfers and Cash Work</td>
<td>(63.1)</td>
<td>(40.4)</td>
<td>(41.1)</td>
<td>(10.2)</td>
<td>(10.2)</td>
<td>(9.7)</td>
<td>(9.6)</td>
</tr>
<tr>
<td><strong>Net Laboratory Funding</strong></td>
<td><strong>467.9</strong></td>
<td><strong>555.9</strong></td>
<td><strong>795.4</strong></td>
<td><strong>590.2</strong></td>
<td><strong>621.7</strong></td>
<td><strong>703.5</strong></td>
<td><strong>631.6</strong></td>
</tr>
</tbody>
</table>

\(^{(a)}\) Does not include proposed construction line item funding for replacement general purpose facilities or new construction programmatic.
D.5 Subcontracting and Procurement

The Laboratory is dependent upon external resources (universities and industry) for support in achieving timely and successful completion of assigned programs and projects. Staff in the Business Support Services organization use the procurement acquisition process in acquiring needed equipment, materials, supplies, and services. The table below reflects actual subcontracted obligations for FY2002 and projections for FY2003 through 2008.

<table>
<thead>
<tr>
<th>Subcontracting and Procurement ($ in Millions—Obligated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fiscal Year</td>
</tr>
<tr>
<td>Subcontracting and Procurement from:</td>
</tr>
<tr>
<td>Universities</td>
</tr>
<tr>
<td>All Others</td>
</tr>
<tr>
<td>Transfers to Other DOE Facilities</td>
</tr>
<tr>
<td>Total Contract 1830 External Subcontractors and Procurements</td>
</tr>
</tbody>
</table>

D.6 Small and Disadvantaged Business Procurement

The Laboratory is committed to support the socioeconomic objectives of DOE and has established procedures and programs that support meeting those objectives.

<table>
<thead>
<tr>
<th>Small and Disadvantaged Business Procurement ($ in Millions—Obligated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fiscal Year(^{a})</td>
</tr>
<tr>
<td>Procurements from Small Businesses</td>
</tr>
<tr>
<td>Procurements from Disadvantaged Businesses(^{b})</td>
</tr>
<tr>
<td>Small Business Goals as a Percentage of Adjusted Annual Procurements(^{c})</td>
</tr>
</tbody>
</table>

\(^{a}\) The year in which a cost appears may be the same year in which the authorization is reported.

\(^{b}\) Procurement from Disadvantaged Business is a subset of Procurement from Small Business.

\(^{c}\) These goals are accumulated based on subcontracts and purchase orders placed with the exception of those dollars awarded to other DOE Integrated Contractors, Battelle Inter-Laboratory Authorizations, other Federal Agencies, State and Local Governments, awards to source directed by DOE, educational institutions, non-profit/not-for-profit organizations, the International Nuclear Safety Program, and firms outside the United States of America.
Appendix E
Laboratory Directed Research and Development: Renewing the Capabilities at PNNL
Appendix E: Laboratory Directed Research and Development (LDRD): Renewing the Capabilities at PNNL

The LDRD program is the principal mechanism for renewing capabilities within the Laboratory and bringing forward novel ideas that will become the next generation of science and technology.

LDRD Program Benefits to DOE and the Laboratory

The LDRD program increases the value that PNNL provides to DOE as a multiprogram national laboratory. Many of the Laboratory's best scientific ideas were developed with LDRD funds and are now contributing to major DOE programs. They include the capabilities and instruments in our Environmental Molecular Sciences Laboratory, high-performance computational software tools that support a broad range of scientific simulations, climate change models, and technologies for immobilizing contaminants in soils and groundwater. Among the most promising new technologies developed under the LDRD program are high-throughput mass spectrometry, advanced microscopic imaging, and cell signaling and protein analyses capabilities that will help DOE and the broader scientific community better understand complex biological systems.

Today, the LDRD program supports the Laboratory in strengthening its base of scientific capabilities. As a multiprogram laboratory serving the challenging requirements of DOE's research and development focus areas, the flexibility provided by the LDRD program allows us to make rapid decisions on projects that address emerging scientific challenges facing DOE missions and to ensure that PNNL remains a modern research facility well into the 21st century.

Institutional Areas of Emphasis

The LDRD program supports new and innovative projects in each of the four research directorates at the Laboratory—Fundamental Science, Environmental Technology, Energy Sciences and Technology, and National Security. Projects cross organizational boundaries and link staff with similar expertise and research interests.

In line with our vision, the following major thrust areas for FY2004 are highlighted below:

Systems Biology and Biotechnology—Enhancing our systems biology and biotechnology capabilities is key to being at the forefront of scientific discovery in life sciences. In particular, the intersection with physics, chemistry, mathematics, and computational science and engineering provides a strong foundation for effective systems biology and biotechnology research. The Laboratory's LDRD projects in this area focus on enhancing fundamental systems biology and applied biotechnology capabilities, particularly as they apply to DOE's Genomes to Life program and the rapidly developing needs in bio-based products.
Computational Science and Engineering— Accomplishment of the Laboratory's ambitious science and technology agenda requires a significant capability in the area of computational science and engineering. We are funding LDRD projects that are building and enhancing our capabilities in areas of computational science, mathematics, and engineering. The goal is to maintain a high-performance computing environment that supports PNNL's key research areas, including atmospheric chemistry and transport, complex biological processes, subsurface science, and materials engineering and simulations.

Nanoscience and Nanotechnology— In addition to building a strong systems biology and biotechnology program, we want to establish a leading presence in nanoscience and nanotechnology with specific emphasis on nano-catalysis and nanobiology. The promise of nanoscience is the ability to design function at the molecular level, and then “teach” those molecules to self-assemble into more complex structures that can interface with biological systems or the macroscopic world. The Laboratory's capabilities in self-assembly, thin-film deposition, oxide synthesis, and molecular modeling will be combined to generate a unique and world-class capability in this revolutionary area of science.

Nonproliferation and Homeland Defense— A number of our LDRD research projects support both Secretary Abraham's emphasis on nonproliferation and homeland defense, and the needs of other federal agencies with interests and responsibilities in this area, such as the U.S. Department of Defense. Our efforts in imaging science and technology are focused on developing next-generation capabilities in image analysis and visualization, which ultimately will be beneficial to a diverse range of disciplines including counterterrorism, nonproliferation of weapons of mass destruction, and materials characterization.

Clean, Secure, and Affordable Energy— We are investigating heterogeneous catalysis, the exploitation of eukaryotic organisms in fermentation and enzyme discovery, and the development of novel reactor and separation systems that will enable us to resolve barriers that currently preclude successful and cost-efficient conversion of biomass into energy and high-value industrial products.

Environmental Quality— In the area of environmental quality, we are conducting research in process science and technology, which is directed toward characterizing materials, improving chemical processes, and identifying new technologies for waste management in ways that increase efficiency, reduce pollution, and perform novel functions. The focus of our efforts is on extending fundamental scientific developments in chemistry and materials to new microscale and conventional-scale systems. The results of this effort can be applied to waste management, environmental cleanup, and carbon management as it affects global climate changes, bio-based products, and processes for energy-intensive industries.

The LDRD Program at PNNL is an important mechanism for ensuring the future strength of our research and technology development capabilities. The program supports investigation of high-risk, high-value ideas. These capabilities and new ideas help the Laboratory to attract the best and brightest scientific staff needed to serve the highest priority DOE mission objectives. It is our principal means for supporting exploratory concepts, innovative approaches, and advanced studies needed to solve the most challenging scientific problems.
Effective Management of PNNL’s LDRD Program

The effectiveness of PNNL’s LDRD program management process is evident by the historical success of its projects. We continue to implement management measures in response to DOE and regulatory requirements.

Schedule

The major sequential steps governing PNNL’s LDRD management process include the following:

May
- The Director of Strategic Planning issues a formal schedule for research proposals, proposal review, and project reporting. Guidance for this process is prepared and issued annually.

May-June
- LDRD proposals are solicited from research staff and selected projects are forwarded to Strategic Planning as candidates for potential funding.

July
- The LDRD Program Office prepares and submits an annual LDRD Program Plan to DOE.

July-August
- The Laboratory reviews LDRD project proposals using both internal staff and external experts.

September
- Recommendations are forwarded to the Research Council for approval.

October
- Principal investigators submit approved LDRD project proposals to the LDRD Program Office for review of compliance with DOE requirements.

October
- The LDRD Office forwards all projects to DOE-AMT for their review and signature for compliance with the DOE Order.

The Laboratory’s Guide to Laboratory Directed Research and Development is a brochure that provides guidance to Laboratory staff and defines the requirements of DOE Order 413.2A. This guide, available on the LDRD internal home page, describes accountability and reporting requirements for LDRD projects and the proper use of LDRD funds. The LDRD Program Office conducts reviews to ensure compliance with these criteria.

Plan

The LDRD Office at PNNL prepares and submits an LDRD Plan to DOE Headquarters that identifies the goals of PNNL’s LDRD program, the broad scientific and technical areas planned for support, the maximum requested funding level, and any requests for fourth-year funding of specific projects.
Peer Review and Self Assessment

PNNL uses peer review to evaluate the quality, relevance, and performance of our scientific research. Peer review is the universally accepted process for determining the direction of and setting standards for scientific, engineering, and technology research and development. The Laboratory has a formal LDRD peer review process that ensures the technical integrity of our work, enhances our stature within the scientific community, and ensures that our research meets our customers’ needs.

Research quality and the potential for research that leads to important scientific developments are best evaluated by employing respected subject matter experts and professionals. The Laboratory uses external peer review panels and conducts an analysis of technical accomplishments as judged by tangible output metrics for LDRD projects. In assessing the performance of LDRD projects, the following criteria are used: technical significance, technical approach, innovation, staff, technical environment, and technical progress. In addition, projects are evaluated to ensure they meet DOE missions and needs. Our review process includes using Advisory Committees, external reviewers for LDRD projects, and Directorate Review Committees.

In addition to technical peer review, the LDRD Program Office reviews projects for compliance with DOE Order 413.2A. Midyear and annual summaries of project performance are analyzed and linked to Laboratory critical outcomes. Project costs and spending rates are tracked in the Laboratory’s financial system. Annual progress reports are obtained from the principal investigators for annual reporting, and tangible output metrics are obtained annually from each principal investigator and analyzed.

<table>
<thead>
<tr>
<th>Laboratory Directed Research and Development Funding (Budget Authorization Dollar Amount in Millions)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2002</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>15.5</td>
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</tbody>
</table>

(a) Estimated  
(b) Proposed
Appendix F
Pacific Northwest National Laboratory Organizational Chart
Appendix F: Pacific Northwest National Laboratory Chart

Pacific Northwest National Laboratory

Laboratory Director’s Office
Leonard K. Peters
Laboratory Director

J.W. (Bill) Rogers, Jr.
Chief Research Officer/ Director, Environmental Molecular Sciences Laboratory

Donald M. Boyd
Deputy Laboratory Director for Operations

Michael J. Lawrence
Deputy Laboratory Director for Campus Development

Environmental Technology
Rod K. Quinn
Assoc. Laboratory Director

National Security
Michael Kluse
Assoc. Laboratory Director

Fundamental Science
Steven D. Colson
Assoc. Laboratory Director

Energy Science & Technology
Michael J. Lawrence
Assoc. Laboratory Director

Human Resources
Paula X. Linnen
Director

Business Support Services
Thomas J. Baranouskas
Director & CFO

Economic Development & Communications
R.M. (Mike) Schwenk
Director

Environment, Safety, Health & Quality
Roby D. Enge
Director

Facilities & Operations
Michael H. Schlender
Director
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