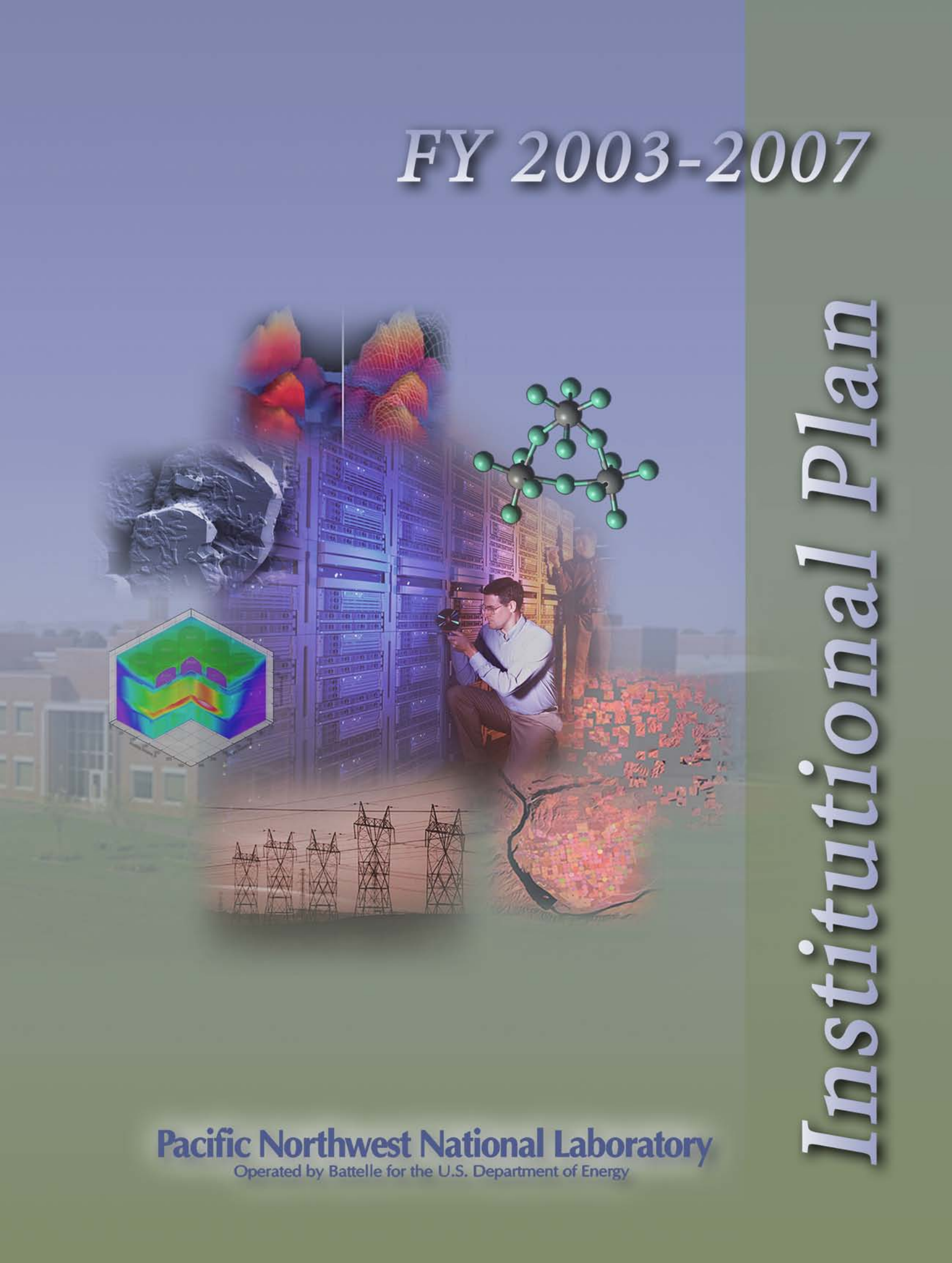


FY 2003-2007

Institutional Plan



Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

About the Cover: Advanced computational capabilities at Pacific Northwest National Laboratory, symbolized by the new Hewlett Packard supercomputer at our Environmental Molecular Sciences Laboratory, support the core strength of the Lab — multi-program science and technology. The companion images on our cover provide a few examples of how our premier computational capabilities (innovative algorithms and software, comprehensive domain knowledge, and high-performance computer systems) promote and enhance our core program research areas.

(Clockwise from top left)

IN-SPIRE, a software tool developed by PNNL researchers, quickly and automatically clusters unformatted text documents together in 3-D format, allowing biologists to uncover common themes and hidden relationships among large amounts of data.

This optimized structure of Sb_3F_{15} represents one of the strongest Lewis acids known. The very high Lewis acidity was discovered based on computations using EMSL resources. Information about such compounds enables scientists to design the synthesis of novel, highly reactive molecules — for example, propellants.

Highly sophisticated computer imaging allows our researchers to develop statistical feature extractions that automatically identify features and segment images into clusters having similar characteristics.

PNNL researchers are looking at energy production and transmission issues to help solve our country's power shortages. An intricate monitoring and controls system, which we simulate on our advanced computers, for the western United States power grid is one of the ways our research is improving energy availability and consumption rates.

High performance parallel computing simulations enable PNNL researchers to perform complex modeling runs that aid in addressing radiological waste storage issues at the Hanford Site.

This scanning electron micrograph shows *Shewanella putrefaciens* CN32 cells on the surface of hematite particles. CN32 is a metal-reducing bacterium important for cycling of carbon and metals in the environment. We simulate shewanella performance in our models of process for bioremediation metals and radionuclides.

Pacific Northwest National Laboratory Institutional Plan FY 2003-2007

April 2003

Prepared for the
U.S. Department of Energy
under Contract
DE-AC06-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

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PACIFIC NORTHWEST NATIONAL LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC06-76RL01830

PNNL-14195



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Director's Statement

The development and publication of this Institutional Plan spans two contract periods (one just expired and another just beginning). During this transition period, PNNL has worked actively with the U.S. Department of Energy and other national laboratories to develop a new management and operating contract that emphasizes results, enhances performance accountability, and provides both the DOE and its contractors with valuable management flexibility. This effort has culminated in a new laboratory strategy, which we believe clearly establishes PNNL's role in providing "Science to Secure America's Future." In helping to realize this future, our broad, multi-program research portfolio will be a central strength that provides outstanding value to DOE. Our 2003-2007 Institutional Plan describes the programs, initiatives, staffing, and infrastructure investments we will pursue in the next five years to deliver that outstanding value.

The plan presents a vision for this contract period that I am pleased to share:

Our Vision

PNNL will be recognized worldwide and valued regionally for our leadership in integrating chemical, physical, and biological sciences to rapidly translate discoveries into applications critical to DOE's missions in energy, national security, and the environment.

Planned Accomplishments in Achieving that Vision

PNNL stands ready in the next five years to deliver exceptional scientific accomplishments to secure America's future, including:

- Establish EMSL and the planned GTL high throughput proteomics facility as world-class research centers for systems biology, physical chemistry, and environmental science, including the stable high-performance computational facility required to enable breakthroughs in these areas of science. The designation of "world-class" will be based in comparison with peers in the international scientific community, on the pace and impact of scientific discovery, and on the reputation of scientists and collaborative user teams affiliated with and/or coming to PNNL to work on scientific grand challenges in the areas of science listed above.
- In the energy mission area, PNNL will develop energy and transportation systems and emission controls to stabilize atmospheric greenhouse gas concentrations, reduce the dollars/kilowatt cost of solid oxide fuel cells for electricity and transportation by 50%, deliver system management tools that dramatically enhance the security, reliability and efficiency of our energy infrastructure, and develop bio-products worth more than \$1 billion annually to our nation's farmers while at the same time reducing America's reliance on foreign oil.



*Leonard K. Peters, Director
of Pacific Northwest National
Laboratory*

- In the environmental mission area, cleanup savings directly attributed to PNNL will exceed \$2.5 billion over five years, ten times the corresponding S&T investment in PNNL programs. PNNL will establish the scientific and technical basis in subsurface science to standardize, streamline, and deploy in situ subsurface treatments that replace costly remediation alternatives.
- In the national security mission area, PNNL will be recognized by the new Department of Homeland Security for its leadership in breakthrough sensing and information technologies that provide highly reliable, early warning detection of the proliferation of weapons of mass destruction.
- PNNL will be recognized as a major economic and educational driver in the region, establishing a post-cleanup presence at Hanford that will accelerate site closure and provide essential S&T for a new and diversified regional economy.

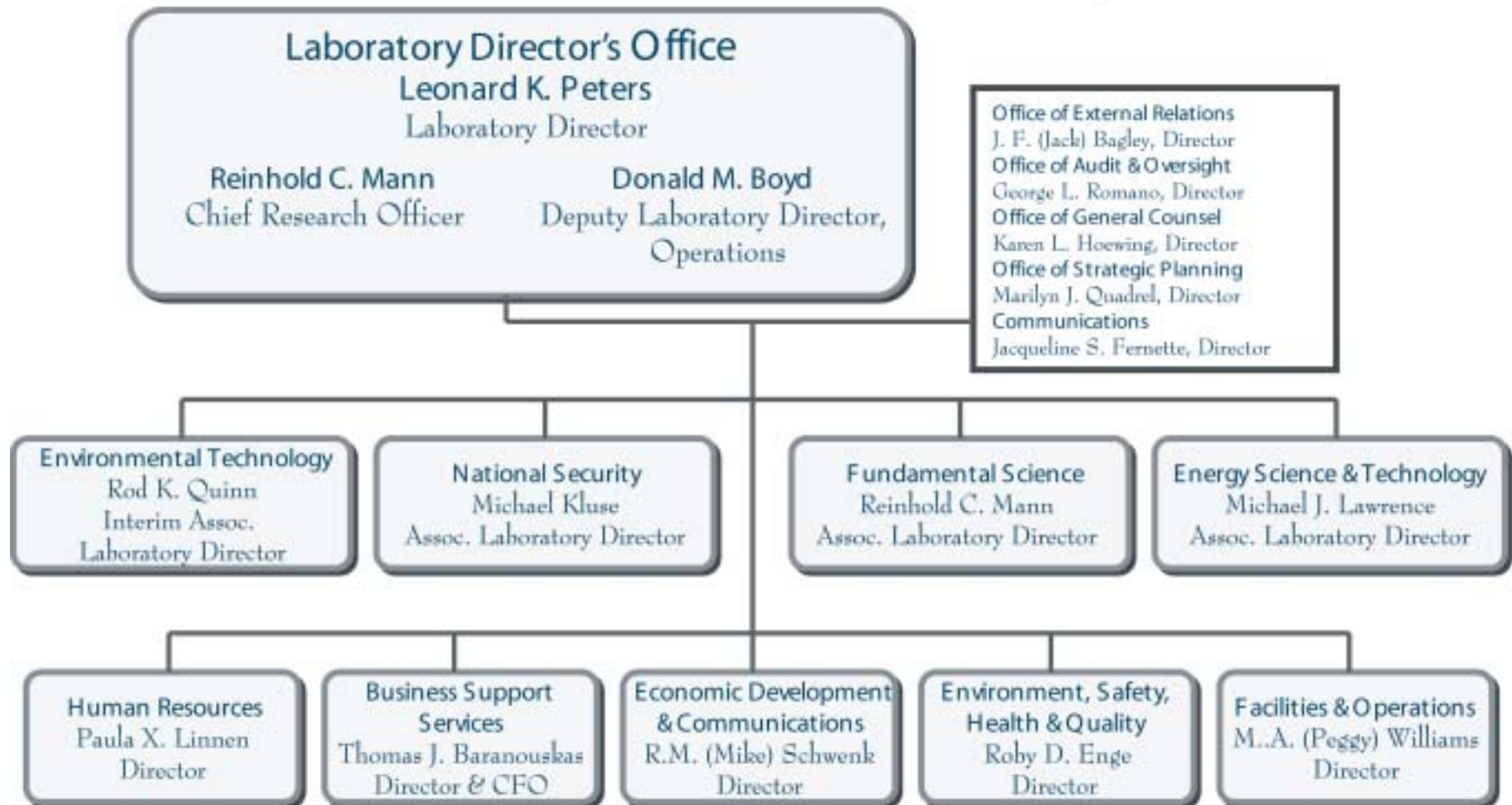
A Transition Plan

This document is a plan for transitioning between the previous PNNL contract and the one yet to be fully negotiated. We expect that parts of this Institutional Plan (e.g., our comprehensive facility plan, operational strategy, and response to Homeland Security) will require adjustment during this next year based on evolving federal needs, identified critical challenges, and the completion of our contract negotiations with DOE.

With the accomplishment of the work described in this plan, PNNL will deliver critical research and forefront scientific facilities necessary to ensure that the DOE can successfully fulfill its core missions, and continues to deliver on the extraordinary promise of science for America's future.



Pacific Northwest National Laboratory



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Laboratory Mission, Roles, and Technical Capabilities

Pacific Northwest National Laboratory is a multiprogram national laboratory that creates new knowledge and delivers solutions to science and technology challenges across all four of the U.S. Department of Energy's missions. Our mission roles are defined by the relationship between DOE's most critical needs and our broad range of research and technical capabilities. That relationship takes shape against a backdrop of shifting global and national priorities, new discoveries in science, and changes in the state of our current capabilities, all of which influence how we target our programs and capabilities to anticipate future as well as current mission needs.

1.1 Mission and Roles

As part of our work under the science mission, we operate the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a national user facility that provides a broad range of advanced experimental and computational tools for advanced research in the environmental, biological, chemical, and materials sciences. Our role in DOE's Biological and Environmental Research programs includes biomolecular science and microbiology, atmospheric science, climate research, subsurface science, and computational modeling. We also conduct significant research programs in chemistry, chemical physics, materials science, nuclear science and technology, and computer and information science as part of DOE's Basic Energy Sciences and Advanced Scientific Computing Research programs. With a systems biology focus, we are building on these current roles to become a significant contributor to DOE's Genomes to Life program. We will expand our user facilities to include new research centers for systems biology and topical computing centers in computational biology, subsurface science, and climate science; and support DOE's overarching mission in national security through expanded classified computation and biothreat reduction capabilities and programs.

In the **national security** mission, we provide science and technology support to DOE and other U.S. government agencies' critical needs to detect, monitor, prevent, and reverse the global proliferation of nuclear, chemical, and biological weapons of mass destruction. We lead international cooperative science and technology programs by applying and developing state-of-the-art technologies and systems to promote nuclear safety, address issues of international security and regional stability, and conduct training for international border security and emergency responders to counter terrorism, both domestically and abroad. We provide science and technology leadership to redirect foreign weapons expertise to civilian applications and to protect or eliminate weapons and weapons-usable materials and infrastructure in the former Soviet Union. Our science and technology also helps ensure the vitality and readiness of the DOE nuclear security enterprise, focusing on critical infrastructure protection and information security.

As the U.S. military transforms to an agile fighting force optimized to the threat environment of the 21st century, we will assist in defining future logistics systems requirements and will develop new technologies to help extend the life of combat systems and ensure a high level of mission accomplishment. We are applying capabilities from throughout the Laboratory to help meet immediate demands for homeland security while investing in new capabilities in advanced sensors and information analytics to meet our nation’s long-term security challenge.

In the **environmental quality** mission, we provide science and technology support to DOE’s waste characterization, waste disposal, cleanup, and land restoration programs, both nationally and at the Hanford Site. Areas of emphasis include vitrification and processing technologies for waste treatment and immobilization, measurements and monitoring, ecological studies, groundwater cleanup, and worker health. New in fiscal year 2002 is the reorientation of DOE’s

Office of Environmental Management’s Science and Technology Program to focus on high-payback, high-risk activities associated with cleanup and site closure. This emphasis will result in transitioning the focus area groups, including the Tanks Focus Area, where the Laboratory has served in a leadership role since 1994. We will support DOE in formulating and managing select focused projects that meet the program criteria, which will include the Hanford, Savannah River, and Idaho Falls sites. We are making focused investments in subsurface science, process science, and worker health that are enhancing our ability to support an accelerated cleanup schedule while minimizing the cost to DOE, its workers, and the public.

In the **energy resources** mission, we provide science and engineering for developing clean, efficient technologies for transportation, energy generation, buildings, and industrial processing. Particular areas of emphasis include lightweight materials for light and heavy vehicles, advanced fuel cell technology, emissions control, advanced nuclear technology, energy systems management, and technologies to improve building performance. We are building on our current programs to enhance our support of the Department’s mission of

providing clean, efficient, and secure energy. These efforts to extend our support include continued investments in carbon management and climate science, bio-based processing, and technology development aimed at transforming the nation’s energy infrastructure.

Pacific Northwest National Laboratory’s distribution of research and development activities by DOE mission area is shown in Figure 1.1. Detailed information about the specific roles and strategies of the science, environmental quality, national security, and energy resources programs at the Laboratory is given in Programmatic Strategy section of this document.

1.2 Technical Capabilities

We rely on the scientific and technical capabilities of our staff to successfully and effectively serve all our missions. We form multidisciplinary teams that draw staff from a wide array of areas of expertise within the Laboratory regardless of their organizational boundaries. This integrated approach to solving scientific and technical challenges helps us apply the full strength of staff capabilities to research priorities.

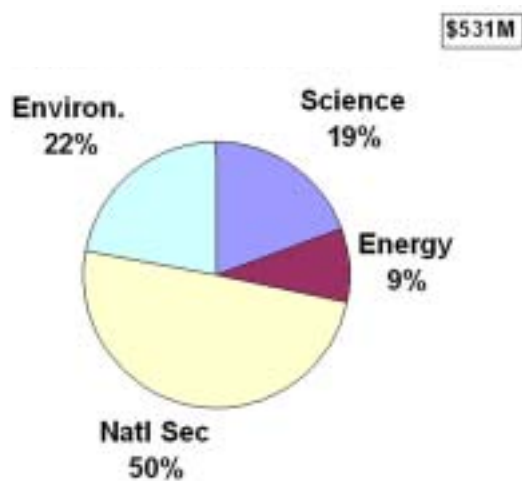


Figure 1.1. FY03 Funding Budget by DOE Business Lines (excl. 1831)

Our signature capabilities and facilities (Table 1.1) serve as the building blocks for our major investments and growing research thrusts in systems biology, computational science and engineering, and nanobiology and nanocatalysis.

These same capabilities enable us to rapidly direct discoveries in our major science focus areas to our programs in national security, energy resources, and environmental quality.

We take specific actions to ensure that our technical capabilities are sufficient, strong, and well positioned for long-term growth.

- Our Laboratory Directed Research and Development program (LDRD), described in Attachment C, is our principal mechanism for supporting exploratory concepts, innovative approaches, and advanced studies needed to solve DOE’s most challenging scientific problems.
- As research areas continue to change in the future, the Laboratory must focus on the future requirements relative to facilities and equipment. Implementation of the PNNL 2010 strategy is intended to align facilities and infrastructure strategies with the major research investment areas. Our facilities strategic plan, although focused, is as dynamic and flexible as the research it supports. Our laboratory operations and management efforts support a strategic facilities plan, which is described in the Site and Facilities Management section. That plan ensures that we have the facilities and equipment needed to attract and retain the best scientists, engage and sustain a broad and productive user community, and realize the scientific discoveries and technology breakthroughs required for a secure nation and thriving economy.
- We form major research partnerships with universities that complement and extend our capabilities, revitalize our staff, and establish an effective vehicle for bringing new talent into the Laboratory.
- We also understand that delivering our vision relies upon truly engaged and fully functional staff and have two vehicles specifically aimed at refreshing

Table 1.1. Signature Capabilities and Facilities

Signature Capabilities	Signature Facilities
<ul style="list-style-type: none"> • Chemical and Molecular Sciences • Process Science and Engineering • Environmental Microbiology, Geochemistry, and Subsurface Science • Environmental and Climate Science • Computational Science and Information Sciences and Technology • Nuclear Sciences and Engineering • Advanced Energy Systems Science and Engineering 	<ul style="list-style-type: none"> • The Environmental Molecular Sciences Laboratory, which includes the <ul style="list-style-type: none"> - Molecular Science Computing Facility - High-Field Magnetic Resonance Facility - High-Performance Mass Spectrometry Facility - Interfacial and Nanoscale Science Facility - Trace Detection Facility - Optical Imaging and Spectroscopy Facility • Microbial Cell Dynamics Laboratory • Cellular Observatory • Gulfstream Aircraft for Atmospheric Monitoring • Atmospheric Remote Sensing Laboratory • Radiochemical Processing Facility • Applied Process Engineering Laboratory • Marine Sciences Laboratory (Sequim, Washington)

and renewing our staff. The first is our technical networks (Table 1.2) that function as internal professional societies for staff to connect with others, expand and update their skills, and align those skills with the requirements of programs conducted across Pacific Northwest National Laboratory and the Battelle-affiliated laboratories. We currently are reviewing the technical networks (see list) to ensure they optimally support the Laboratory's growth agenda and our DOE programs. The second vehicle is a Gallup program aimed at understanding and increasing staff engagement in the Laboratory's missions. We conducted a baseline Gallup survey in fiscal year 2002 and will be following up on those results with Gallup-designed programs to increase staff engagement. Annual follow-up surveys will help us gauge our progress and redirect our efforts as appropriate.

Table 1.2. Technical Networks

- | | |
|--|--|
| <ul style="list-style-type: none">• Analytical and Physical Chemistry• Biosciences and Biotechnology• Computational Science and Engineering• Computer Science and Information Technology• Design and Manufacturing Engineering• Earth System Science• Energy Technology and Management | <ul style="list-style-type: none">• Human Health and Safety• Materials Science and Technology• Nuclear Science and Engineering• Policy and Management Sciences• Sensors and Electronics• Separations and Conversion• Statistics. |
|--|--|

Laboratory Strategic Plan

Last year, Pacific Northwest National Laboratory initiated a comprehensive revision of our laboratory strategic plan. This section of our FY 2003-2007 Institutional Plan describes our point of departure and approach to forming PNNL 2010, our 10-year vision and strategy for the Laboratory. In summary, our vision is to be a best-in-class U.S. Department of Energy Office of Science multiprogram national laboratory with internationally recognized capabilities and facilities for systems biology and biotechnology research. We will perform research and development at the interfaces of the biological, computational, and physical sciences to deliver innovative and effective solutions to critical national and societal challenges that cross all four of DOE's missions. We will achieve this through our outstanding staff, demonstrating leadership in research and development and in laboratory operations, and delivering high value to our customers, community, and the region.

We will continue to refine and sharpen this vision to reflect our new contract and external changes. This section outlines our Laboratory Agenda and action plan for achieving this vision.

2.1 Key Planning Assumptions

Our vision and action plan for this 5-year period are based on some important assumptions concerning mission priorities and programs, science and technology opportunities, policy and budget variables, and institutional challenges.

2.1.1 Mission Priorities and Programs

DOE's mission priorities and programs will continue to be shaped by significant global and national trends, as articulated below

In **science**, multidisciplinary, mission-oriented research laboratories and agencies will need advanced capabilities in systems biology, computational science, and nanoscience and nanotechnology for the next 5 years and beyond to fulfill their missions. Specifically:

- Applications of biotechnological advances will be critical to meeting challenges in areas from sustainable, clean energy supply to defense against biothreats. The ability to make use of genome sequence information and to apply advanced analytical technologies to observe and measure processes in vivo are key to understanding, mimicking, and safely exploiting the fundamental processes in living organisms and their interactions with the environment.
- High-performance computing will become increasingly central to progress in many areas of science and engineering. Major scientific advancements will come from researchers who are part of interdisciplinary teams combining expertise in experimental science; theory, modeling, and simulation; and computational science.

- The ability to observe and manipulate matter at the nanometer scale will provide new tools and technologies that will advance the chemical and material sciences with resulting impact on all DOE missions.

We assume that the Office of Science Genomes to Life and computational science programs will grow into significant programs to support these drivers.

DOE's missions will be affected by the Department's overarching priority on **national security**. Homeland defense will continue to be a national priority as reflected in the nation's new Homeland Security Department. The science agenda supporting this priority will include a focus on biodefense, a demand for broad and reliable detection of all threats, a concomitant requirement for effective information analysis, and a requirement for rapid and secure communications at all levels of government. Nonproliferation of weapons of mass destruction will continue to remain a priority for both homeland defense and national security.

Demand for clean, affordable, and secure energy will grow in parallel with concerns for homeland security. Security concerns regarding reliance on imported oil, increased domestic energy consumption, and a growing consensus about global warming will drive continued interest in alternative energy sources, including fuel cells, bio-based production, and nuclear energy. An increasing demand for energy will come with an increasing requirement for more reliable and efficient infrastructure. Technology suitable for transforming our existing infrastructure will become more available and affordable and the demand and desire for a more flexible and responsive infrastructure for deploying these communication-rich technologies will grow. We assume that the Department's Energy Efficiency and Renewable Energy and Fossil Energy programs in fuel cells, bioenergy, and climate change will grow, and that the Nuclear Energy programs will remain viable.

In **environmental quality**, the desire to accelerate the cleanup and establishment of long-term security of former weapons production sites while minimizing cleanup costs will continue to drive a demand for advanced science and technology to enhance cleanup processes, protect workers, and ensure states, communities, and other stakeholders of the viability of the Department's long-term solutions. DOE's Environmental Management programs will remain funded and focused on closure of the cleanup mission.

2.1.2 Scientific and Technical Opportunities

Researchers at the Laboratory are positioned to make important discoveries and inventions in the rapidly developing fields of systems biology, high-performance computing, and nanobiology and nanocatalysis.

Systems biology and high-throughput proteomics. Recent achievements in sequencing the human genome and detailed knowledge of a growing number of other important genomes open new opportunities for the Laboratory in systems biology and biotechnology. Our strengths in microbiology combined with high-throughput mass spectrometry and magnetic resonance spectroscopy will allow us to characterize the proteome (the population of proteins encoded by the genome) in living cells, and understand changes induced by stress responses and functional characteristics of individual proteins and protein complexes.

Computational science. The successful high-performance computing center in chemistry and molecular sciences at Pacific Northwest National Laboratory is a

model for effective application of terascale computing to enable scientific discovery. It combines strong expertise in computer science and applied mathematics with scientific domain expertise and represents a dedicated high-performance computing resource for a significant user community. A commitment to maintain a cutting-edge terascale (and beyond) computer system at the Laboratory combined with growth in programs such as Genomes to Life, SciDAC, and applied missions will provide the means to establish additional topical centers focused on biology, subsurface science, and regional climate modeling.

Nanobiology and nanocatalysis. Nanoscience and nanotechnology will revolutionize many areas of science and technology, with potential applications in electronic devices, novel smart materials, chemical processing, heterogenous catalysis, and the molecular components of living cells. Before the promise of nanoscience can be realized, two primary challenges must be addressed—designing and manipulating molecular-scale structures, and assembling these nanostructures into functioning systems capable of interfacing with the real world. By applying the Laboratory’s strengths in soft materials interfaces; synthesis; theory, modeling, and simulation; and characterization, we are building a strong scientific foundation that will bring benefits across all our missions and programs.

Our ability to direct discovery in these areas to mission applications rests on our ability to make advances in a host of additional areas, including

- Physical chemistry
- Information visualization
- Statistical analysis
- Subsurface science
- Environmental, atmospheric, and climate science
- Sensing and imaging methods
- Measurement science
- Advanced instrumentation.

We assume that we will be able to continue to make Laboratory Directed Research and Development investments within the Department’s new guidelines for the program. We assume that we will have the flexibility to steward our facilities and equipment in ways that allow us to streamline our management activities and reinvest resulting savings to renew our capabilities.

2.1.3 Policy and Budget Outlook

We assume that DOE’s overarching national security mission will result in continued support for fundamental science, advanced energy technology, environmental quality, and national security research and development. We believe that federal science and technology budgets, including DOE research and development funding, should at least be stable and may increase, perhaps substantially, during the next 5 years. This view is based on broad recognition by Congress and the new Administration that investments in research and development underpin U.S. technological leadership, stimulate growth in the national economy, and provide solutions in the war against terrorism. We anticipate enduring support for funding for life and environmental sciences, growing budgets in the physical sciences, and growth in homeland and national security-related research

and development. Energy research also may see growth, as this aspect of national security has significant ramifications on the future of the U.S. economy. Even if optimistic projections prove accurate, the environment for allocating resources will be highly competitive with essentially every state government seeking to create forefront research universities and attract other research investments as a means to sustainable economic growth. The Office of Management and Budget guidelines for making federal investment decisions in basic and applied research and development 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 productivity.

2.1.4 Institutional Challenges

We are addressing several institutional or management challenges in order to successfully realize our vision for the next 5 years.

- ***Recruiting and retaining staff in a highly competitive environment.*** Two trends are affecting our ability to attract first-rate research staff. First, the increasing speed with which scientific discovery is translated into commercial advances is creating new and extraordinary opportunities for researchers, particularly in high-growth areas such as information technology or biology. Second is the ongoing and well-known demographic change in the U.S. workforce, with an increasing share of that workforce coming from demographic groups traditionally underrepresented in science and engineering. To compete successfully, we must provide a high-quality work environment, including outstanding facilities and equipment, intellectual freedom, and the opportunity to contribute to significant outcomes. In order to be recognized as an employer of choice for technical professionals, we will need to provide incentives and benefits, intellectual challenges, and opportunities for advancement and scientific leadership to an increasingly diverse workforce.
- ***Ensuring forefront facilities and equipment.*** Revitalizing our aging facilities and constructing modern research laboratories is absolutely necessary if Pacific Northwest National Laboratory is to maintain first-rate research capabilities. Substantial capital investment in new buildings and equipment will be needed. Obtaining these investments given constrained funding and vigorous competition will remain a substantial challenge throughout the next decade.
- ***Building effective partnerships with other research institutions to solve major national challenges.*** We must form productive partnerships to bring the full suite of required research capabilities to critical national needs. Through our cadre of top-level scientists and strategic partnerships with universities, other laboratories, and industry, the Laboratory must increase its role as a regional and national resource.
- ***Creating visibility, advocacy, and ownership to attract programs and investment.*** Given the substantial competition for funding that we foresee, strong support and advocacy from the scientific and university community as well as from our local community and region will be essential to realize our agenda. This advocacy can be developed only through outstanding performance that leads to recognition of the Laboratory as a critical research asset.

2.2 Achieving Our Vision: Laboratory Agenda

As a result of the PNNL 2010 planning effort, we identified five strategic objectives that we must meet to successfully realize our vision in light of today's challenges and opportunities. We must achieve science and technology excellence, recruit and retain outstanding staff, demonstrate leadership in operations, deploy beneficial technologies and contribute to the region. These strategic objectives are the vehicle for implementing our commitment to simultaneous excellence, and they provide the overall framework for our Laboratory Agenda.

Each year, the Laboratory Agenda is reviewed and revised according to management consensus on the actions considered most important. As we begin developing our fiscal year 2003 Laboratory Agenda, we will outline specific actions that we will be pursuing in the near term and ensure that those actions directly align with the overall objectives in PNNL 2010. The Laboratory Agenda is the basis for our annual mission and business planning and is widely available to staff on an internal website.

2.2.1 Science and Technology Excellence

Objective

As a preeminent research organization, Pacific Northwest National Laboratory seeks excellence in science and technology as we advance the frontiers of science, deliver extraordinary research tools, and provide science-based solutions for DOE's missions in national security, environmental quality, and energy resources. Our critical roles in each mission depend on a strong foundation in fundamental science. We continue to rely on our basic research and expect the new knowledge provided by these efforts to leverage our programs across the Laboratory.

Key Outcomes

- **Create a leading systems biology and biotechnology program.** Pacific Northwest National Laboratory will be recognized for our multidisciplinary approach and valuable contributions to biotechnology research and development. Establishing comprehensive biosciences capabilities will lead to substantial program growth with DOE and the National Institutes of Health, and scientific discoveries that will benefit all mission areas. As we expand our systems biology and biotechnology programs, we will focus on the goals of DOE's Genomes to Life program, on biothreat reduction, and on bio-based products and processes to enhance sustainable production and energy independence.
- **Maximize the scientific impact of the Environmental Molecular Sciences Laboratory's user program** by using a new approach that will bring communities of users together around EMSL's distinctive capabilities to address major scientific grand challenges. Building on the base of their substantial scientific accomplishments, EMSL's users will initially focus on biology and subsurface science, expanding to additional areas such as atmospheric science or catalysis. The expanded group of users will be using a best-in-class user operational model assembled from user facilities across the DOE complex.
- **Play a leadership role in building the nation's high-performance computing capability** with an emphasis on applying tera-scale computation and simulation science to some of the most pressing questions underlying DOE's science, national security, energy, and environmental missions. We

are conducting efforts that optimize the integration of new mathematical and statistical approaches, high-performance software, advanced operating systems and high-performance computers, and extensive domain knowledge to address challenges in computational molecular science, computational biology, subsurface science, and physics-based climate simulation.

- **Be a leader in detection and analysis technologies for homeland and national security** by applying new science and technology solutions for infrastructure protection, counterterrorism, arms control, and nonproliferation and defense needs. Our capabilities in this area will support the prevention of proliferation of all types of weapons of mass destruction and the detection of nuclear, chemical, and biological threats to our people, cities, economy, and national assets. We will be recognized as a leading Office of Science laboratory for providing impactful solutions to the National Nuclear Security Administration's nonproliferation mission. We will lead nontraditional approaches to global security by addressing the root causes of global conflict. We will improve the safety of nuclear power generation and the management and disposal of nuclear material in the former Soviet Union.
- **Become a science and technology leader in secure, clean, and affordable energy** by delivering breakthrough energy generation and management technologies that reduce our reliance on foreign oil, reduce the negative environmental impact of energy production, and enhance the reliability and cost efficiency of our energy infrastructure. We will provide a balanced portfolio of energy solutions including energy efficiency programs, power systems, and carbon management systems. We will deliver science and technology for developing clean, lightweight, and efficient vehicles including specialized materials and emissions technologies, advanced, cost-effective solid oxide fuel cells, and biobased fuels and products. We will provide the basis for setting new directions for our energy infrastructure. We will provide leadership in understanding and mitigating the impacts of climate change.
- **Be the leading science and technology laboratory for expedited cleanup and sustainable process** by delivering innovative and cost-effective solutions to DOE's legacy cleanup program and to the management of regional and global environmental resource conflicts. We will support environmental monitoring and measurement needs and provide expertise in policy and management decisions relating to environmental impacts and health risks. We will significantly advance our understanding of contaminants and how they affect the environment and humans. We will increase the efficiency, reliability, and safety of cleanup processes, and we will develop new knowledge and technologies that protect worker safety. To address environmental concerns and management of national and global resources, we will identify sustainable solutions for global economic development and explore processes for cost-effective production of chemicals and materials from renewable and sustainable feedstock.

2.2.2 Outstanding Staff

Objective

Every aspect of our vision requires the effort and dedication of our staff. To be successful, we must attract, develop, and retain outstanding staff and managers. Highly engaged managers and staff are highly productive, have high operational

efficiency, and contribute substantially to the Laboratory's missions. Through talent-based selection and development programs, we will create an environment where staff members are well positioned to help realize our vision. Our leaders, managers, and staff will be recognized as best in class, indicated through peer reviews and external comparisons.

Key Outcomes

- **Demonstrate that managers and staff are highly engaged** through objective measurement. We will annually measure staff engagement and implement actions and changes that will increase engagement. We will correlate engagement with productivity and communicate observed best management practices throughout the Laboratory.
- **Earn recognition as an employer of choice for research** by enhancing management and staff selection, succession planning, diversity, integration, education, and external recognition; maintaining impactful programs and state-of-the-art facilities and equipment; and providing helpful management systems and infrastructure.

2.2.3 Laboratory Operations and Management

Objective

We will be recognized as a benchmark for streamlined laboratory management and operations that facilitate excellence in research. To do this, we must develop and implement innovative approaches that enable high-impact research while becoming the most cost-effective national laboratory. This will require implementing management systems that anticipate and respond to changing program needs; ensure safety, security, and other requirements through processes that are embedded in our daily work; progressively increase scientific productivity through improved work practices; and develop and maintain forefront research facilities and equipment.

Key Outcomes

- **Provide new and revitalized facilities that enable research and development** for solving our customers' most pressing scientific and engineering challenges. This effort includes seeking new partnerships and funding sources for continued renewal.
- **Increase science and technology productivity** through innovative work practices. During the next few years, we will have systems in place that are fully consistent with the new DOE-Headquarters research and development performance metrics. Our researchers and operations staff will be among the world's most productive according to external standards. The impact of our users and user facilities will be among the highest in the DOE laboratory system.
- **Demonstrate outstanding operational performance** of our management systems. We will establish model contract performance measures and best-in-class standards for all management systems. We will pursue an overall cost-management strategy including incentives and appropriate productivity and cost metrics. And, we will share management systems and best practices with other laboratories and establish a reward/recognition process for positively impacting operations at Pacific Northwest National Laboratory or other laboratories.

2.2.4 Beneficial Deployments

Objective

Technologies developed at Pacific Northwest National Laboratory are broadly available for, and deliver high value to, DOE and other governmental missions, and provide substantial social and economic benefits to the region and the nation. It is critical that we reinvest and regenerate the means for conducting research and development. Our commercialized technologies generate substantial returns for reinvestment in Laboratory staff and infrastructure. Our technological advances also drive business growth by attracting new customers and enhancing our reputation for rapidly translating discoveries into business applications.

Key Outcomes

- **Deploy technologies that result in major benefits** to DOE and other government agency missions as well as to the economies of the nation and region. We will increase the number of deployments by the Laboratory and by our clients or partners and enhance communications about these successes.
- **Earn commercial returns to refresh the Laboratory**, which includes re-engineering the commercialization business model to accelerate the return of discretionary income from intellectual property to the Laboratory. Other actions that will boost financial returns involve increasing staff and management participation in the commercialization process, determining the funding level needed to mature technologies and protect intellectual property, and revisiting the recognition and rewards program for staff.
- **Demonstrate sustainable growth and diversification** to achieve an increase in available resources for reinvestment and renewal. Growth in our core and new business areas is essential to providing new opportunities to staff and the resources necessary for new capabilities and process improvements. An ongoing study will address hiring issues, shift investment strategies toward markets with the highest potential, and identify successful business strategies and means to increase investments in capabilities.

2.2.5 Valued Regional Asset

Objective

We will be known for our contributions to solving the region's important technical challenges, local and regional economic development, regional science education, and the quality of life in the community. As an integral part of the region's science and technology network, we want to be recognized as a trusted and valued collaborator and partner and to earn local and regional support and advocacy.

Key Outcomes

- **Make substantial impacts** that improve the quality of life and overall prosperity of the region. We will support higher-education enhancements, assist and support local and regional firms, partner with Northwest entrepreneurial programs, and pursue opportunities to support partnerships, entrepreneurial activities, and community involvement programs.

- **Garner broad advocacy that attracts investment** in new programs and capabilities. We will extend and enhance our interactions with regional government and industrial leaders to build this advocacy. We will focus on building scientific user and community advocacy for a systems biology facility, a bio-based products facility, and higher education enhancement.

2.3 Summary and Path Forward

Our approach to strategic planning has changed in the last year as we shift from developing our ten-year strategy to implementing that plan. For the first time, all our planning activities have a single reference point in the PNNL 2010 action plan, outlined above. Our fiscal year 2003-2007 critical actions will follow the strategic objectives in that plan, which we consider a living document. Both the strategic objectives and key outcomes may change over time. However, our intent is to use this as a framework for strategic planning and assessment. It will guide performance-based measures for the 5-year period of our new contract and our future submissions of the Institutional Plan.

3

Major Laboratory Initiatives

Laboratory science and technology research initiatives^(a) strengthen our ability to respond to current and anticipated U.S. Department of Energy mission needs. These initiatives ensure that Pacific Northwest National Laboratory remains well positioned to provide a high level of science capability and responsiveness to DOE's research and development priorities. Our major initiatives are also designed to leverage programs in all of DOE's primary missions. Over time, successful initiatives transform into significant new DOE research programs, with new capabilities that also may benefit other existing programs. The knowledge, tools, and scientific competencies that emerge from successful initiatives often lead to new scientific or technical opportunities.

Our Biomolecular Systems initiative is working toward major goals of the Genomes to Life program^(b) and is developing new tools intended to facilitate a systems approach to biology. Our Computational Sciences and Engineering initiative will develop significant new tools for multidisciplinary research for "A New Era of Scientific Discovery through Advances in Computation."

Other initiatives are directed toward supplying the science and technology base needed for science, energy, environmental, and national security mission requirements. Our Nanoscience and Nanotechnology initiative is creating capabilities for basic research applications, tools, and materials that support all of DOE's missions. Our initiative on Carbon Management will lead to technology that contributes to stabilizing atmospheric carbon dioxide levels supporting the Energy Resources core mission and contributing to the implementation of the President's climate change initiative. Our Imaging Science and Technology initiative is developing advanced technologies for characterizing land features and environmental conditions from aerial and satellite data sets. This technology also has exciting applications in medical and biological imaging. The completed Infrared Sensing initiative developed sensors to detect and identify chemicals associated with national security threats with beneficial applications in environmental research and resource management.

In line with the Office of Science's energy resources mission needs, our Bio-Based Products initiative will provide new catalysis and fungal processing technologies for

The Office of Science's research priorities provide a framework for our initiatives



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Biomolecular Systems	Page 3.3
Computational Sciences and Engineering	Page 3.11
Nanoscience and Nanotechnology	Page 3.18
Bio-Based Products	Page 3.23
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Imaging Science and Technology	Page 3.28
Energy Systems Transformation	Page 3.31
Advanced Nuclear Science and Technology	Page 3.33

- (a) Initiatives are provided for consideration by the Department of Energy. Inclusion in this Plan does not imply DOE approval of or intent to implement an initiative.
- (b) Genomes to Life: Accelerating Biological Discovery, DOE/SC-0036, April 2001. All publications are downloadable from the website: DOEGenomesToLife.org.

converting agricultural products and wastes into modern fuels, which support the priority to develop and ensure rapid application of evolutionary and revolutionary new sources of energy for the future. Our Advanced Nuclear Science and Technology initiative will contribute to the reinvigoration and refocusing of nuclear capabilities and will help develop next-generation nuclear power system components and controls, which support the President's national energy plan to increase production from domestic sources. Our Energy Systems Transformation initiative will develop creative new ways to manage key electrical transmission systems for more efficient energy distribution supporting the DOE priority to revolutionize conservation and energy efficiency. Our completed Fuel Cell Technology initiative supports DOE's efforts to ensure abundant and clean energy. This initiative integrated new materials and designs into high-density configurations that can be manufactured cost-effectively as energy sources for both stationary and mobile applications, which supported the development and assurance of rapid application of evolutionary and revolutionary new sources of energy for the future.

A major emerging initiative for the Laboratory is our **Homeland Security Initiative**. Pacific Northwest National Laboratory has been contributing to reducing the global threat of terrorist or state-sponsored use of weapons of mass destruction for many years. However, the September 11th attacks on America have forever changed our understanding of the horrific nature of the terrorist threat, as well as the advancements in science and technology that are needed to enable us to discover, detect, and prevent similar events in the future. In response to this national need and the daunting scientific and technological challenges it poses, the Laboratory is launching a new initiative in Homeland Security in fiscal year 2003. The strategic outcomes of the initiative are focused on developing greatly improved methods of early threat detection and prevention. The science and technology agenda is focused on advanced sensor and information technology. The initial Laboratory Directed Research and Development investments related to this initiative will be made in two areas:

- **Detection**—Advanced materials and sensors for improved collection, separation, and detection of chemical, nuclear or biological agents including improved methods for analyzing multiple sensor data sets to identify subtle threat indicators with lower false alarm rates. Research in this area strongly leverages advancements and capabilities being developed in the Nanoscience and Nanotechnology Initiative, the Computational Science and Engineering Initiative, the Biomolecular Systems Initiative, and the Advanced Nuclear Science and Technology Initiative.
- **Knowledge Discovery**—Development of new analytical, statistical, and computational methods to discover relationships about potential threats by processing enormous and diverse information sets including documents, measurements, images, financial transactions, internet traffic, and other data types. This will require breakthroughs in multi-dimensional information synthesis, scenario and hypothesis-driven analysis, new methods for human-information interaction, and automated software tools for anomaly detection, threat recognition, and uncertainty calculation.

Our long-term strategy for homeland security also includes leadership in evaluating the efficacy and implementation trade-offs of proposed technology solutions. The creation of a Technology Testing and Evaluation capability is an integral part of our strategy to be involved in the full range of activities from scientific research

In fiscal year 2003, Homeland Security will emerge as a major new initiative, focusing on early threat detection and prevention.

through technology implementation. Our involvement in research and implementation will provide a well-founded understanding of the needs and problems that will enable us to assist DOE and other government agencies with overall homeland security policies and risk management strategies. Specific objectives and thrusts in these areas will be developed through the course of fiscal year 2003. Promising areas will then be considered for midyear funding and for the fiscal year 2004 initiative plan.

In addition to developing critical new capabilities needed for homeland security, this initiative will integrate and focus many capabilities from across the Laboratory, particularly from other Laboratory-level initiatives, on this important national priority. At the same time, the scientific and technological advancements resulting directly from this initiative in the area of separations, sensors, and information analysis will have broad applicability to other DOE mission areas such as biological and chemical research, bio-processing, and environmental management.

3.1 Biomolecular Systems

Building on the extraordinary capabilities in the William R. Wiley Environmental Molecular Sciences Laboratory and the Laboratory's prominent program in microbiology, the Biomolecular Systems initiative will provide an integrated framework and set of tools for tackling complex problems in biological systems that can be solved only by work at the interface among disciplines. Research under this initiative is directed toward the major goals of DOE's Genomes to Life program.

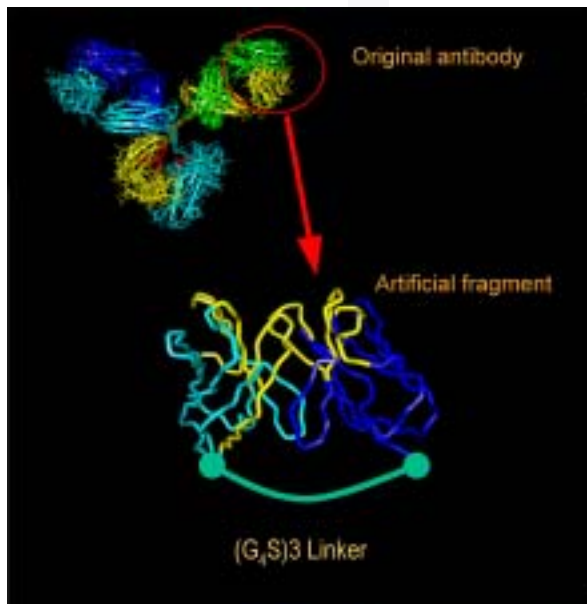
The completion of the sequencing of the genome presents new challenges and opportunities in the biological sciences. The genome specifies the potential proteins in a cell whereas the proteome is the actualization of that potential. Proteins are components of molecular networks that control the inner workings of living cells. To understand the function of genes, we must understand how they work as parts of molecular networks. The goal of the Biomolecular Systems initiative is to understand the interactions of biomolecules within cells from a systems perspective to determine how intracellular protein networks regulate cell responses to the extracellular environment. This knowledge can provide fundamental insight into biological pathways and will allow us to understand roles that individual genes play in living cells and how to manipulate cell behavior for useful purposes.

The joint DOE and National Institutes of Health Human Genome Project has identified the base-pair sequences that make up about 30,000 genes in human DNA. The next step is to determine the functions of these genes by analyzing the proteins or protein subunits that are encoded by these genes. These materials interact to implement various functions of life. The current challenge is to identify the vast number of proteins encoded by the genome and how these proteins interact to carry out essential processes in living cells. To meet this challenge, the initiative is employing a multidisciplinary strategy that integrates proteomics, imaging technologies, and computational modeling to understand the metabolic and regulator networks within cells. We are defining the cellular proteome using high-throughput mass spectrometry, isolating and identifying protein complexes, visualizing proteins in time and space using novel optical instruments, and using the data in conjunction with computer simulations to



Pacific Northwest National Laboratory is investing in a multidisciplinary, collaborative research program that integrates molecular biology, biochemistry, physics, mathematics, and computer science to advance our understanding of complex biological systems in the post-genomic era.

simulate cell behavior. The aim of our research program is to understand the mechanisms that control a cell's response to its environment. This will help scientists predict how cells respond to environmental stimuli or injury and how to control these responses. This research may lead to important discoveries of the function of microbes and cells and the causes and potential treatments for several human diseases.



The new Single Chain Antibody technique developed by Biomolecular Systems Initiative researchers enables the creation of high-affinity probes suitable for detecting pathogens and cancer-associated proteins.

The Laboratory investment in advanced systems biology builds on and extends the one-of-a-kind facilities and instruments in the Environmental Molecular Sciences Laboratory. The Laboratory has built a significant program in proteomics and has demonstrated leadership in high-throughput mass spectrometry. We are also developing the next-generation instruments for direct observation of chemical and physical processes in living cells.

Computational biology and informatics are also central to our capability development efforts. Informatics is necessary to collect and interpret the high volumes of data generated by proteomics technologies. Tool-based delivery systems are needed to support molecular dynamics and reaction chemistry. Tools for modeling cellular behavior are needed to integrate multiple cellular processes into predictive frameworks. We are also building the biological program that can exploit these advanced instruments and facilities so that these technological advances can be applied to meet needs important to DOE.

Our biological sciences program is directed at understanding carbon sequestration and energy production by microorganisms as well as the human health effects of low-dose exposures. It also

is well aligned with the DOE environmental quality mission and its attention to worker and public health risk assessment and to environmental remediation. It addresses the national security mission by facilitating our understanding of the consequences of chemical and biological weapons, and by developing new approaches to detect bioterrorism threats. It is also directed to the energy resources mission needs for clean and affordable power and efficient and productive energy use.

Our vision of further discoveries in systems biology that will be enabled by these tools, in conjunction with the resource needs identified in the May 2002 Genomes to Life "DOE Resources and Technology Centers for Biological Discovery in the 21st Century" report, serves as the driving force behind plans for systems biology research centers at Pacific Northwest National Laboratory. These centers will complement the Environmental Molecular Sciences Laboratory and its capabilities at the interface of the physical, life, and information sciences.

3.1.1 Research Strategy

Systems Approach to Intracellular Networks. Understanding how cells respond to their environment from a systems perspective is a major focus of the Biomolecular Systems initiative. All living cells sense and respond to their environment by a complex set of biochemical mechanisms. These mechanisms are part of a complex system of communications that govern basic cellular activities

and coordinate the actions of cells. Before researchers can understand the behavior of cells, they must understand how these biochemical networks operate.

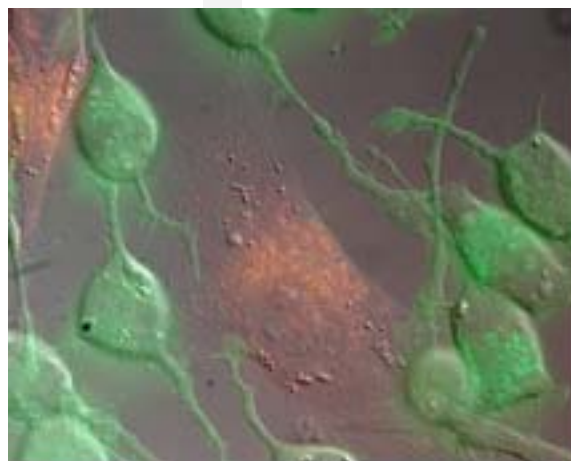
Signaling networks must be understood as complex, integrated systems. The initiative is developing new technologies and approaches to accomplish this task. Cells receive information from their environment through different classes of proteins, such as receptors. The information is then processed through signaling pathways and decoded in the nucleus and other areas of the cell. Understanding cell signaling is dependent on knowledge of spatial and temporal dynamics for receptors and signaling pathways. The initiative team will investigate which pathway components are present in a given cell, where the components are located, and the functions that these components perform.

A systems perspective of the whole cell requires describing the system in terms of measurable parameters. Thus, a quantitative approach to biology is key to our success. Important cellular parameters, such as protein-protein interactions, can be quantified using biochemistry, mass spectroscopy, and imaging. Databases and computer models will be needed to handle the large amounts of data that will be generated by quantitative, high-throughput assays. The process of investigating and delineating cell-signaling pathways will require the simultaneous application of many capabilities by multidisciplinary teams of scientists.

We have developed models of information and metabolite processing in cells using a combination of a top-down and bottom-up approach. Signaling and metabolic networks are modeled as a series of interacting modules composed of defined groups of proteins. The interactions of these proteins are described in terms of rate constants and their spatially restricted concentrations. These models will be experimentally tested by using high-throughput proteomics to determine the proteins that are present in responsive cells and the concentration of relevant species. Imaging technologies will be used to determine the interaction of proteins and their spatial localization. Data from these high-throughput technologies can then be compared to model predictions, resulting in the development of more accurate models. This cycle of theory, experiment, and analysis is an essential component of modern science. The complexity of biological systems, however, requires a corresponding increase in the complexity of the theory, the volume of data, and the power of the analytical techniques. In addition, because cells change their pattern of protein expression in response to changes in conditions, cells must be maintained under closely controlled and documented conditions. Thus, systems biology requires a very tight integration of theory, experiment, and analysis.

Systems Biology Research Centers: Capabilities, Resources, and Facilities.

With the Laboratory's growing expertise and the capabilities and resources available in the Environmental Molecular Sciences Laboratory, we have made significant progress in solving many of the difficult technical issues associated with the generation, capture, and analysis of high-throughput biological data. It is important to create research environments that allow the coupling of experimental design to the resulting biological data. Laboratories investigating a common problem should be linked, either physically or virtually, with a set of shared models, a common set of techniques, and coordinated research agendas. Biological research will benefit



In Pacific Northwest National Laboratory's Cellular Observatory, researchers are working to improve their predictions of protein interaction.

In its May 2002 Genomes to Life “DOE Resources and Technology Centers for Biological Discovery in the 21st Century” report, DOE identified the required resources and facilities to carry out the Genomes to Life program. Consistent with this report, Pacific Northwest National Laboratory proposes to provide systems biology research centers consisting of capabilities, resources, and facilities to engage in cutting-edge research in systems biology.

by moving toward the more integrated research models practiced in other scientific fields, such as chemistry or physics. New and enhanced resources for the application of high-throughput technologies to important problems in systems biology will significantly accelerate progress in the field.

Research critical to the core missions of both DOE and the nation will be conducted in laboratories that also will support the continued development of instrumentation and technology. These proposed systems biology research centers will promote the interactions necessary for conducting systems biology at the Laboratory with high-speed data links necessary to provide a virtual link to other research laboratories in the Department of Energy and academic organizations. We anticipate that these new centers will serve as a hub for conducting systems biology for many purposes. They will operate as user facilities, providing scientists from academic institutions, other national laboratories, and industry with access to previously unobtainable instrumentation and resources. These new facilities will be built on our experience of creating the Environmental Molecular Sciences Laboratory and our current efforts focused on making it the leading user center in environmental science at the molecular level. Collaboratory software and high-speed Internet connections will allow users to perform experiments remotely. Data collected both remotely and within the facilities can be integrated into a more comprehensive understanding of biological systems. The integration of these systems biology research centers will provide DOE with a premier advanced systems biology capability to address DOE’s missions in the 21st century.

The long-range goals of the Genomes to Life program will result in the establishment of national resources that contain capabilities and technologies necessary to achieve the program goals. The systems biology research centers proposed by the Pacific Northwest National Laboratory will accommodate an integrated suite of unique, state-of-the-art experimental and computational capabilities. One potential research center, the Production Proteomics Facility, will house high-throughput instruments for protein production and protein array research supported by a strong bioinformatics and computational biology infrastructure. Available to users, this center will include unique capabilities in data visualization and analysis.

The critical technologies this proposed center addresses are complex, require a large support infrastructure, benefit from increased scale, and are beyond the reach of most biological research laboratories. The most critical of these technologies were developed and continue to be advanced at Pacific Northwest National Laboratory. A strong core team exists and substantial investments in infrastructure already have been made.

Other possible research centers include capabilities in molecular imaging and subcellular localization being developed in the initiative’s Cellular Observatory. The Cellular Observatory will provide the capacity for an expanded user community to use state-of-the-art optical microscopy instruments to collect real-time data on multiple cellular functions and across scales of space and time. Some instruments will enable research at the molecular level while others will be focused on microbial communities and tissues. For example, the Microbial Cell Dynamics Core Laboratory is in the early demonstration stage of integrating flexible experimental systems capable of making multiplexed measurements of cellular responses and processes under relevant environmentally controlled conditions.

To support an integrated user facility concept and promote collaborative research, the Biomolecular Systems initiative is bringing together teams from partner universities, other national laboratories, and industry. Constituencies are being formed to identify resources necessary to advance scientific instrumentation and technologies to meet emerging research needs and support a resource concept directed toward systems biology research.

3.1.2 Topical Research Areas of Emphasis

The Biomolecular Systems initiative's five key enabling components all are directed at understanding cellular networks. These components are designed to complement each other and to provide the necessary technologies to build a systems biology enterprise. Within the **Proteomics** area are one-of-a-kind mass spectrometry capabilities that catalog and characterize proteins on a large scale, allowing rapid identification of proteins made in response to changes in the cellular environment.



The William R. Wiley Environmental Molecular Sciences Laboratory plays a critical role in reaching the goals of the Biomolecular Systems Initiative.

A high-throughput single-chain antibody facility allows the generation of affinity reagents for protein isolation and identification with unprecedented speed. In the **Cellular Observatory**, sophisticated optical and magnetic resonance instruments can follow molecular processes in living cells. The spatial localization of biomolecules can be determined and their biochemical microenvironment can be investigated. In the **Computational Biology** area, computer simulations are being created to build complex hypotheses of cell behavior. Advanced, mechanistic models of cells allow us to create high-throughput hypotheses to evaluate the ever-expanding mass of biological data. The **Bioscience Software** program is building software tools to handle data obtained from complex biological systems. Bioinformatics tools will allow the collection and analysis of distributed data sets. Collaboratory software will allow teams of biologists located at sites throughout the world to work together productively. The **Environmental Microbiology** program is developing approaches to understanding carbon and energy flow in complex microbial communities. Understanding how bacteria communicate and regulate their energy metabolism is key to controlling their behavior and designing new approaches to bioremediation and renewable sources of energy.

Proteomics. Much of the understanding of cellular systems and the role of their constituents will come from the newly emerging field of proteomics. The proteome is the entire complement of proteins expressed by a particular cell, tissue, or organism at a given time under a specific set of environmental conditions. The greatest challenge for proteomics research is to rapidly measure the proteome using small amounts of tissue or cultured cells. An additional challenge is to measure the interaction of large sets of proteins. To address these critical issues, we are developing technologies that include: 1) advanced mass spectrometry and experimental techniques that provide a systems-level view of the entire proteome,

2) protein array technologies using highly specific recombinant antibodies to identify critical steps in cell regulatory networks and to characterize functional protein complexes, 3) microfluidics-based protein biomolecular interaction assay systems for quantitative observation of interactions and determination of relevant thermodynamic and kinetic parameters, and 4) a protein production laboratory for cloning, expressing, and purifying milligram quantities of active proteins and antibodies for functional and structural studies. These capabilities will not only allow us to characterize the composition of cells, but will provide data and tools necessary to understand the dynamic regulation of cells.

Cellular Observatory. Visualization of protein distribution and dynamics can be a powerful tool for understanding protein functions. To exploit this potential, we are developing a capability with multispectral instruments that allow proteins to be visualized in a functional context. These instruments will be used to investigate both isolated protein complexes and complexes within living cells.

The prototype microscopes under development in the Cellular Observatory include

- *Single-Molecule Microscopes.* These instruments are capable of seeing single molecules, allowing real-time investigation of proteins binding to specific substrates.
- *High-Speed Fluorescence Resonance Energy Transfer Microscope.* This new instrument is a high-speed, multiwavelength microscope that will investigate the dynamics of protein-protein interactions in living cells. By using fluorophores with overlapping excitation and emission spectra, the interaction of molecules can be followed.
- *Coherent Anti-Stokes Raman Scattering Microscope.* Laser frequencies in this microscope can be set to excite signals from cell membranes or other cellular structures with unusual spectral characteristics as well as visualize fluorescently labeled proteins. This allows the localization of proteins in the context of a specific intracellular environment.
- *Patch-Clamp Optical Microscope.* This instrument provides correlated optical (molecular scale) and ion channel activity (cellular scale) on the same isolated segment of a cell membrane in a living cell. This instrument will allow the first direct measurements of the time and spatial relationships that control these important cell membrane processes.
- *Optical/Magnetic Resonance Microscope.* This instrument combines simultaneous cellular and multicellular magnetic resonance imaging and spectroscopy with confocal imaging.

Computational Biology Program. Data from proteomics studies or from the Cellular Observatory will be used to build mechanistic simulations of biological systems. Biological processes are inherently hierarchical. Events at the molecular level initiate actions that result in complex biological outcomes at the cellular, tissue, and organ levels. The Biomolecular Systems initiative's Computational Biology Program is designed to simulate complex biological processes spanning the molecular level to the macroscopic level of organization. This program provides the integration for our systems approach to biology.

At the level of finest detail, researchers are investigating how small molecules interact with proteins to lead to signaling events. The role of protein-protein interactions in controlling cell-signaling pathways is investigated using techniques



The Pacific Northwest National Laboratory is developing capabilities with multispectral instruments that allow proteins to be visualized in a functional context.

from computational chemistry. At another level, researchers consider the cell as a three-dimensional structure, similar to a chemical plant that consists of many complex unit processors. The overall architecture and appropriate structural and functional modules are designed, tested, and integrated to create effective models. Synthesizing multiple temporal and spatial scales of interest requires massively parallel computers, data storage systems, networking, and software.

To keep pace with the post-genomic sequencing era, new capabilities are needed to efficiently interpret the vast amount of DNA sequence data being deposited in public and private databases. Computer software is being developed to evaluate expression analysis data. Software has been developed to display the information graphically so that large volumes of data can be readily visualized. The initiative also is developing and integrating credible biophysical models for processes occurring at the molecular and cellular levels. These models are being integrated into exposure-to-dose response models for organs and tissues. Our goal is to develop an organ-level biophysical model beginning at the cellular level to realistically predict the frequency of early genotoxic events created in simulated organs and tissues by endogenous processes, low-level ionizing radiation, and man-made chemicals.

Bioscience Software. Software development and information technology play a major role in the Biomolecular Systems initiative and crosscut the other components of the program. Information architecture will bridge the areas of research and facilitate a systems approach to biology. The goal is to develop the underlying infrastructure for scientists to support ongoing research and transform the work environment with tools necessary to do multidisciplinary science. Information technology promises to substantially enhance the productivity of the biological research enterprise.

We are developing the following capabilities: 1) applications that support data acquisition, data management, visualization, and analysis needs with an organized approach at handling data; 2) data and information management to formulate management strategies, storage solutions, and interfaces to data and information and to provide an overall infrastructure necessary to support the Biomolecular Systems initiative's research agenda; and 3) collaboratory software to integrate and develop tools necessary to support ongoing collaborations and problem solving and provide an integrated environment for scientists, as well as supporting access and manipulation of complex data sets and facilitating the interactions between researchers, peers, and students. The initial project is to develop and integrate software and processes to acquire, manage, and analyze data streams from the optical instruments within the Cellular Observatory. This software environment will form the foundation for the next generation of tools for handling high-throughput data generated by the technologies that underlie the Biomolecular Systems initiative.



PNNL researchers are advancing our environmental microbiology capabilities in:

- *rapid removal of technetium in ground waters*
- *characterizing the proteome of Deinococcus radiodurans*
- *understanding the mechanisms of metal and radionuclide reduction by D. radiodurans R1*
- *understanding the syntropic relationship between the fermenting bacteria and methanogenic organisms.*

The Biomolecular Systems initiative provides opportunities for expansion into other program opportunities, including those of the National Institutes of Health, the Department of Defense, and the biotechnology industry.

Environmental Microbiology. The Biomolecular Systems initiative links the Laboratory's expertise in environmental microbiology with capabilities in molecular and computational sciences. Our goal is to develop capabilities to investigate microbial communities from a systems perspective. We will investigate fundamental processes involved in metal reduction, carbon fixation, methanogenesis, and other mechanisms involved in the production or conversion of energy.

Microorganisms play critical roles in human health and the environment. They also represent the largest pool of genetic and biochemical diversity on the planet. A wealth of gene sequence information is now available for an ever-increasing number of microbes. However, little is known about microbial gene expression and the function of specific genes in microbes' native environment, or how cells respond to stimuli using sensory mechanisms and regulatory networks. Recent scientific evidence suggests that gene expression patterns and regulation can be radically different in laboratory cultures as compared to the native microbe habitat. Thus, to understand the basic function of microbial cell pathways, it is necessary to observe cells under environmentally relevant conditions.

To address this necessity, the initiative is supporting the development of a new Microbial Cell Dynamics capability within the systems biology research centers concept. This capability will offer a flexible and highly controlled instrumented experimental system and allow the investigation of microbial cells under a range of environmental conditions (mixed cultures, nutrient status, and extremes of pH, temperature, salinity, radiation, and light). It also will allow us to simulate the environment from which the microbes were originally isolated in order to understand molecular-level processes in a biologically relevant content.

3.1.3 Role in the DOE Research Agenda

The Biomolecular Systems initiative supports the DOE overarching national security mission to better understand biological mechanisms relevant to microorganisms and the human health effects of low-dose exposures. In addition, it will further discoveries in advanced technologies and computational models for use in the biological sciences. Powerful new observational instruments as well as advanced computation and modeling will be required to attack fundamental questions of biological mechanisms and effects at the molecular and cellular levels.

The research projects in the Biomolecular Systems initiative are aligned with the Department of Energy's newly announced Genomes to Life research program. Genomes to Life is a joint program with the Office of Biological and Environmental Research and the Office of Advanced Scientific Computing Research. This partnership, represents a 10-year program plan in systems biology, using whole genome DNA sequence in combination with DOE resources to address complex molecular networks in organisms that allow them to respond to and interact with their environment. Proteomics and microbial systems will be major components of the Genomes to Life program, which began with the DOE Microbial Cell Project.

The Biomolecular Systems initiative is well aligned with the environmental quality mission and its attention to worker and public health risk assessment, and to environmental restoration. Some of the project areas are focused on understanding gene regulatory networks and cell signaling pathways involved in microbial responses to environmental stress, such as radiation or heavy metals. This information will be crucial in modifying the behavior of microorganisms to

facilitate their use for bioremediation in environmental cleanup. Work also is under way in building computer-based models for extrapolating the effects of radiation and chemical exposure. Molecular sensors are being built for the evaluation of both worker exposure and for the rapid detection of potential biowarfare and bioterrorism agents. These basic research efforts also address the needs of the national security mission to understand the consequences of chemical and biological weapons, and the needs of the energy resources mission for clean, affordable power and efficient, productive energy use.

3.2 Computational Sciences and Engineering

Computing has revolutionized the way that we live and the way that we practice science. Together with analytical theory and experimentation, computational science has developed into the third branch of science bridging the other two. Computational science and engineering will be the key to many of the advances that will occur in science during the 21st century. As examples, it has recently become possible to solve the complex equations that describe natural phenomena at accuracies that are comparable to, and in some cases, better than those available from experimental measurements. It also has become possible to perform sophisticated analyses on the prodigious amounts of information coming from today's experimental and remote sensing devices.

Computational science and engineering play a key role at Pacific Northwest National Laboratory and will continue to do so in the future.

Our focus is on key areas relevant to the Department of Energy missions where we have demonstrated capabilities and excellence. Computational science is a vital element of the Department's missions as it allows us to derive new understanding about complex phenomena across temporal and spatial domains. Today, computational science at the Laboratory is being successfully applied to DOE's science, energy, security and environmental quality/remediation missions. As the role of solving the equations that describe natural phenomena more and more accurately on high-performance computers increases in the scientific enterprise, we must continue to build our capabilities for this third leg of the scientific triangle.

For Pacific Northwest National Laboratory to maintain its core science programs, meet the mission needs of the Laboratory, and to build for its future role, we must be among the world's premier computational science institutions, helping to lead the journey to effective application of petaflop computing to solve real scientific and technical problems in focused areas. The Laboratory must also continue to contribute substantially to the theory and practice of computational science and engineering. Computation will be an integral part of essentially every element of the Laboratory's research – from chemistry and biology, to energy utilization and security, to environmental management, to national security. To accomplish this objective, we propose an ambitious effort to enhance our core computational science and engineering capabilities.



At Pacific Northwest National Laboratory, we employ advanced theoretical approaches implemented in high-performance software on massively parallel computer systems to advance our fundamental understanding of science and technology.

We propose to build our computational science program around the idea of focused research efforts in specific application areas (in terms of the Scientific Discovery through Advanced Computing plan, Topical Computing Facilities). Our core science areas are:

- computational molecular science with a focus on basic science including molecular structures, reaction energetics and kinetics, and spectroscopy with applications to environmental science, interfacial science, catalysis, biochemistry, and nanoscience;
- computational biology with an emphasis on systems biology including whole cell modeling and using large data sets from high throughput experiments;
- environmental science with applications in atmospheric chemistry, regional climate modeling, and subsurface reactive transport with a focus on the DOE-wide vadose zone issues; and
- national security.

We intend to either lead or be a major partner in Topical Computing Facilities in biology, subsurface reactive transport, and regional climate in addition to our core Topical Computing Facility, the Molecular Science Computing Facility in the William R. Wiley Environmental Molecular Sciences Laboratory with its focus in chemistry, biochemistry and biophysics, environmental science, and nanoscience. Most of the computer time to the Molecular Science Computing Facility is allocated to Computational Grand Challenge teams which are groups of computational scientists from across the scientific research complex who are trying to solve very large and complex problems by using the most advanced hardware and software.

We plan to support the above focused application areas with core expertise in specific areas of computational and applied mathematics and computer science. Our core areas in computational and applied mathematics are discrete mathematics and combinatorics; grid development and solution methods; the development of high-performance scalable algorithms based on multi-resolution analysis; and how to handle uncertainty in modeling and simulation. In computer science, our focus is on providing and advancing the computer science foundation for developing high-performance scalable and portable computer codes and operating system software for both present and future massively parallel computing systems, and distributed computing environments such as computational grids including network security; and developing the base infrastructure and middleware for the construction and maintenance of discipline-specific collaborative problem-solving environments.

Computational science and engineering will be the key to many of the science advances during the 21st century. As such, it plays a key role in many of the Laboratory's other initiatives, including Biomolecular Systems, Nanoscience and Nanotechnology, Energy Systems Transformation, Carbon Management, and Imaging Science and Technology. For example, the efforts in the Computational Sciences and Engineering initiative provide essential elements of the base technology for the computational aspects of advanced biology and nanoscience research, as well as nuclear power simulations, optimized electrical power distribution, and advanced imaging technologies.

As part of a national user facility, access to the Molecular Science Computing Facility is 100% open to scientists who pass a detailed peer review process whether they are staff at Pacific Northwest National Laboratory or at a university, national laboratory or industry.

3.2.1 Research Strategy

The goal of our internal investments in computational sciences and engineering is to address mission needs through the use of high-performance computing by intimately coupling hardware and software with advanced algorithms and domain-specific methods to address complex problems. This initiative focuses on

- developing high-performance, portable, and scalable algorithms and software for massively parallel computer systems
- developing the associated computational infrastructure, including high-performance parallel computing tools and frameworks, advances in operating systems for improved performance on massively parallel processor computers, scalable visualization and analysis techniques, and middleware for collaborative problem-solving environments
- developing an applied mathematics and statistics infrastructure coupled to the computational science effort to support the computational science effort
- applying computational sciences to selected DOE mission areas, focusing primarily on basic science, environmental, energy, and national security issues.

These investments have positioned the Laboratory to support major DOE Office of Science computational science initiatives, including the Scientific Discovery through Advanced Computing (SciDAC) initiative, the Genomes to Life program, and initiatives from the FreedomCAR and Vehicle Technology Office. A key component to our vision is the development of topical computer facilities as noted in the SciDAC plan. The prototypical SciDAC topical computing facility is the Molecular Science Computing Facility in the Environmental Molecular Sciences Laboratory. The Molecular Science Computing Facility combines high-end massively parallel hardware; high-end software (Molecular Science Software Suite or MS3); a graphics and visualization laboratory; user support, consulting, and system operations services including operating system modifications and development; and a large-scale data archive and scientific data management system. The Molecular Science Computing Facility has just signed a contract to install a next-generation Linux cluster supercomputer from Hewlett-Packard with peak performance of 9.1 teraflops, 3.8 terabytes of memory, and 173 terabytes of disk storage. This new architecture will be incorporated, as appropriate, as part of the DOE's Ultrascale Simulation Computing capability. The Ultrascale Simulation Computing capability will incorporate a variety of different computer architectures including a Cray X1 vector-based computer at Oak Ridge National Laboratory and advanced Power and Blue-gene computer systems from IBM at Lawrence Berkeley National Laboratory and at Argonne National Laboratory. In addition, there are a number of potential advanced architectures being proposed by a variety of vendors including Hewlett-Packard which can be investigated by a broad DOE national laboratory partnership. We will support the Ultrascale Simulation effort by making our computers available to the community for benchmarking and testing of software as a function of machine architecture and will also benchmark and test our software on new computer architectures at other laboratories. In addition, we propose to expand our efforts in developing the ParSoft suite of tools for parallel computer architectures to these advanced architectures. An Ultrascale Simulation computing capability will enable dramatic new scientific advances in a variety of areas ranging from computational catalysis and nanoscience to computational

We have established a significant degree of commonality in the leadership teams of the various initiatives and in the management of staff to fully integrate all aspects of the computational science that are being carried out at the Laboratory.

biology to subsurface modeling to climate modeling. As an example, Ultrascale Simulation computing systems could be used for a Cell Simulator with a focus on whole cell simulations, extensive genome-wide comparisons of large numbers of genomes with a goal of examining both phylogeny and gene regulatory networks, and modeling the dynamics and functions of protein complexes—the molecular machines of life.

The development of topical computing facilities involves the integration of hardware with optimized software in a single facility tuned to the needs of a specific scientific or engineering domain so that the highest possible performance is achieved as well as allowing the most complex scientific problems to be addressed. A key goal is to be the home or play a major role in topical computing facilities in specific domain areas appropriate to the Laboratory's mission including biology, subsurface science, and atmospheric sciences/regional climate in addition to the Molecular Science Computing Facility. The Laboratory's investments are designed to strengthen our capabilities in the areas of computational modeling and simulation that are critical to our long-term goals including the underlying infrastructure in computer science and mathematics. To meet these goals, investments are being made in the following key areas of strategic Laboratory interest with a focus of providing new capabilities to serve as the nucleation point for additional Topical Computing Facilities.

Computational Biology. The emphasis is on developing and applying new computational and mathematical tools for systems biology, in collaboration with other Laboratory investments in this area. Tools are being developed for genomics and proteomic data analysis leading to the development of cellular models, modeling cell-signaling pathways in realistic cellular systems including the use of discrete mathematical approaches and advanced kinetics solvers, protein-protein interactions by using molecular simulations, reconstructing cells to get high spatial resolution models based on microscopy data, developing models of cellular communities, and biological data analysis and mining. A key signature of our computational biology effort is a close interaction between computational biologists and chemists, experimental biologists and chemists, mathematicians, and computer scientists. This effort is closely aligned with the Department's Genomes to Life program, with a specific focus on microbial cells.

Subsurface Science. The emphasis is on developing high-fidelity reactive transport codes applicable to a wide range of pollutant transport problems in the subsurface including the vadose zone at the Hanford Site. Significant success has been achieved in developing new methods implemented in high-performance software for massively parallel architectures that are being used to address reactive transport in the Hanford vadose zone. This software has specific applications for the Office of Science's EM Science Program, as well as for the cleanup program at Hanford. The software for massively parallel computers will enable scientists and engineers to develop state-of-the-art models that include as much detail as possible in order to predict the fate and transport of contaminants through the vadose zone as reliably as possible. This will enable scientifically defensible and site-specific predictions of contaminant fate and transport for critical waste management and cleanup decisions.

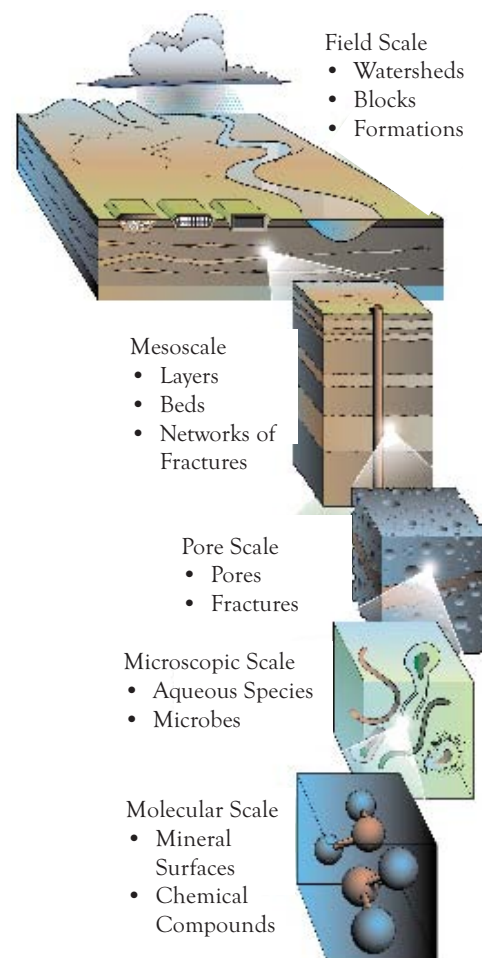
Climate Change. The Laboratory will continue to develop its capability in regional climate modeling. We will develop the tools needed to understand how global climate change affects critical environmental resources and the human

activities that depend upon them in regional areas both in the United States and in countries important to U.S. interests. Understanding these types of problems requires information at temporal and spatial scales that are beyond the capabilities of current global climate models as well as the kinds of global models that will be developed within the foreseeable future. In addition to developing improved regional climate models, we will also be developing improved models that can be used as a test bed for generating and evaluating the next generation of high-resolution climate models, including better physics in cloud models and subgrid models. We also are developing new atmospheric chemistry models implemented in high-performance software that can be used, for example, to model intrusion of stratospheric ozone in small regions or to look at aerosol formation. We are continuing to support our efforts in computational chemistry through programmatic work and by additional LDRD investments. Computational chemistry has been a core strength of Pacific Northwest National Laboratory since the founding of the Environmental Molecular Sciences Laboratory and we are growing our capabilities in this area.

Chemical Sciences. The emphasis is on improving the performance and capabilities of the award-winning NWChem code for the types of thermochemical, chemical kinetics, and spectroscopic calculations broadly needed for addressing DOE's missions in science, energy, environment, and national security. Significant advances have been made in developing new coupled cluster methods including treatments of open shells and implementing these methods in NWChem. This progress will allow us to investigate the reactions of the much larger molecules that are of key interest to a broad range of DOE mission areas. In addition, advances in nucleation theory are being supported with a focus on the formation of aerosols, a broad topic covering many of DOE's mission areas.

The Laboratory has had a long history in providing resources to protect the nation and we are continuing to make investments in this key area which has become even more important since 9-11.

National Security. Imaging science plays a key role in all aspects of science and technology—from data formation and analysis to decision-making, from laboratory instruments to new satellites, and from the molecular and cellular scale to the global scale. Current serial algorithms and tools for image analysis are not adequate for the scale of today's problems—and future requirements will be even more demanding as our ability to acquire large data sets grows. New analysis methods, computational approaches, and integrated decision support tools are needed that can use massively parallel computers. Advanced image analysis algorithms and methodologies are being developed in collaboration with the Imaging Science and Technology initiative. Our Computational Sciences and Engineering initiative is developing parallel software for image-to-image registration, boundary determination, calibration, and data fusion that will provide significantly increased capabilities and throughput. Also, computational chemistry capabilities and programs have important applications in actinide science and radiation materials science at the molecular scale including reactor design. Such computational chemistry tools can be used in the design of chemical and biological warfare detection systems, in actinide science and radiation materials science, and as an aid in guiding the remediation of contaminated sites.



Advanced subsurface simulators allow researchers to incorporate scale and uncertainty into models.

Underlying the above five application areas are our investments in the core infrastructure in computer science and applied mathematics. Integrating applications with advances in computer science and mathematics has been a key signature of the Laboratory in computational science.

Computer Science. The emphasis is in two key areas: 1) providing the computer science basis for high-performance scalable and portable computer codes and operating systems for present and future massively parallel computing systems including distributed computing systems, and 2) developing the base infrastructure and middleware for the construction and maintenance of discipline-specific collaborative problem-solving environments for regional climate modeling, computational chemistry, atmospheric chemistry, computational biology, and engineering simulations. As part of this effort, we have been developing new approaches to data analysis and visualization of large model and experimental data including the development of novel data signature techniques. Developments in the underlying technologies and middleware common to all collaborative problem-solving environments, such as new web-based database technologies, also have been made. Our goal is to have a strong fundamental computer science group with a basic research focus on high-performance computing and the development of problem-solving environments whose expertise can be leveraged in the development of software for specific application domains.

Applied Mathematics. The emphasis is the development of a fundamental science effort in applied mathematics with a focus on discrete mathematics and combinatorics, grid and solution methods, and the development of high-performance parallel computing algorithms both general, such as eigensolvers, and for specific domain application areas. Progress in building up this area has been made through key new hires. Discrete mathematics is an important technique for computational biology, national security, and energy systems applications, e.g., power grids. The focus on adaptive mesh technologies and the underlying mathematics was established to provide the best description of the physics for the most realistic geometry of the model system. The new codes, NWGrid (grid generation) and NWPhys (physical equation solvers), are being developed as the P3D system for massively parallel computer systems, and already have been applied to a growing list of problems in chemistry, biology, and engineering.

Software Infrastructure. We are continuing to enhance our paradigm for software development based on teams. Our team approach to software development is based on our successful development of the award-winning Molecular Science Software Suite (MS³) for computational chemistry, initially funded under the Office of Biological and Environmental Research and the Office of Advanced Scientific Computing Research Computational Grand Challenge program in high-performance computing. A crucial component of this successful effort was the teaming of computer scientists, applied mathematicians, application developers, theoreticians, and users (domain scientists) in designing and implementing the software. This approach results in synergy that enables development of the highest-performance software with the best algorithms that is scalable, portable, and has the longest in-use lifetime. Such teams also help to minimize long-term development costs by producing software that is, to the maximum extent possible, portable and readily maintained and updated. These factors are especially important when tackling the many grand challenge computational problems faced by DOE. Our approach to software development is a key capability that we bring to DOE as it

Our focus in applied mathematics is the development of a core basic research effort that can be leveraged to support the development of new computational methods in specific domain areas.

advances its agenda in computational science. In addition, we bring a capability in delivering high-performance computing cycles in an efficient and usable manner to a focused user base in terms of topical computing facilities.

Hardware Infrastructure. Planning for multi-teraflops scale topical computing facilities requires a focus on the next generation of massively parallel computers and the associated software development needed to drive new applications, as well as for the gigabit networks and infrastructure to support such computers and applications for a national user base. Science drivers for the new hardware and software include:

- computational molecular science with a focus on basic science, including molecular structures, reaction energetics and kinetics, and spectroscopy including applications to interfacial science, catalysis, and nanoscience;
- computational biology;
- environmental science with applications in atmospheric chemistry, regional climate modeling, and subsurface reactive transport with a focus on the DOE-wide vadose zone issues; and
- national security.

High-bandwidth, low-latency networks that support differentiated services will be a critical component for any teraflops computing center and a critical capability to support major computational activity for a broad user base that is geographically distributed. In addition to supporting this initiative, high-performance networking will benefit other initiatives and will position the Laboratory for other work requiring high-performance electronic communications capability, and will support the goal of expanding and supporting the user communities who will access these resources.

3.2.2 Role in the DOE Research Agenda

Scientific simulation makes defining contributions to almost every area of science and engineering. The efforts of this initiative are strongly tied to the missions of DOE with a focus on the Office of Science priorities as described in the S1 Mission Review's Information from Pacific Northwest National Laboratory, prepared by the Office of the Director, dated 11/30/01; and Dr. Raymond Orbach's testimony to Congress dated 3/15/02.

- Efforts are being made to develop capabilities to 1) improve our ability to model combustion processes beginning at the molecular level and going to the macroscopic level; 2) improve modeling of metals, ceramics, and advanced materials; 3) improve our ability to design catalysts from first principles with a focus on energy production from fossil fuels; 4) improve our ability to predict how aerosols form both in combustion systems and in the atmosphere; and 5) mathematical/computational models of electric power grids.
- Our efforts are focused on helping to clean up the environment by providing tools to understand the fate and transport of contaminants in the subsurface and in the atmosphere from a variety of anthropogenic sources. We are developing new tools to aid in minimizing pollution and energy use in chemical production processes, as well as for the design of new materials for environmental cleanup and restoration. In addition, we are developing computational biology tools that will enable us to better understand how microbes can be used to remediate contaminated sites.

We are planning and deploying the network and infrastructure required to support the next generation of simulation and computing activities at Pacific Northwest National Laboratory.

- The software being developed in the Laboratory is critical for modeling simple and complex systems with a broad range of applications including those in molecular chemistry, biology, environmental science, and energy use and production. These tools will let us explore larger molecules in significantly more detail than previously possible, and will make accurate computational thermochemistry, kinetics, and spectroscopy a reality. A significant effort is under way to investigate the fundamental relationships involved in the behavior of systems at different spatial and temporal scales that underlie the behavior of complex systems.
- Efforts are focused on providing groundbreaking applications based on advances in software, computer science tools and libraries, mathematics and statistics, and the base computational infrastructure to solve complex problems on the world's fastest computers.

3.3 Nanoscience and Nanotechnology

New opportunities created by nanoscience will revolutionize many areas of science and technology. Because of these new opportunities, scientific management will be faced with the significant challenge of choosing which areas are appropriate to pursue, consistent with developing strong basic science and supporting the applied mission areas of the Department of Energy. The machinery itself, in the form of enzymes and nucleic acids, operates at the nanoscale and the leveraging of scientific breakthroughs from the Genomes to Life Program with new smart nanomaterials promises paradigm-shifting improvements in key mission technologies such as detection, catalysis, and remediation.



Scanning electron microscope (SEM) picture of Al₄C₃ nanoribbon. Scientists at Washington State University and Pacific Northwest National Laboratory have discovered that Al₄C₃ nanoribbons were formed at relatively low temperatures. Nanoribbons are a new variety of synthesized nanostructures, and may lead to a wide variety of technological applications such as inexpensive ultra-small sensors, “smart” windows for controlling the amount of heat and light entering buildings, and other functional devices with low-power consumption and high sensitivity. This work was highlighted by Science as a surprise development in this area.

The apparently inexorable advance of Moore’s law^(a) in semiconductors now suggests that 30-nm transistors may become reality by 2015. Fabrication of devices at the nanoscale using variations of the “top down” approach developed throughout human history and applied so successfully by the semiconductor industry is unlikely to be effective and still less likely to be commercially viable as the capital cost of chip fabrication equipment soars. At the scale of a few nanometers, design at the molecular level followed by assembly of those molecules into devices, as envisioned by Feynman^(b), comes into its own. For the first time in history, we are beginning to design from the “bottom up.” A major federal initiative in nanoscience and nanotechnology is under way to accelerate the development of this young field of study.

Beyond electronic devices, the breadth of nanoscience makes it an intrinsically interdisciplinary area that is an essential foundation for the future research needs of the Laboratory, including novel smart materials, chemical processes, electronics, and the molecular components of living cells.

- (a) Moore’s law, proposed in 1964 by Gordon Moore (co-founder of Intel Corporation), is the observation that the logic density of silicon integrated circuits doubles approximately every 18 months.
- (b) Richard Feynman (Nobel Prize in physics, 1965) “There’s Plenty of Room at the Bottom: An Invitation to Enter New Field of Physics,” December 29, 1959, at the annual meeting of the American Physical Society.

Many distinctive and potentially useful properties emerge as feature sizes approach the nanoscale, including transport properties (momentum, energy, and mass) that evolve from a continuum to a molecular description and optical, electrical, magnetic, and chemical properties that cross over from a classical to a quantum description. By manipulating matter on a nanometer scale and taking advantage of changes in these physical properties and using hierarchical assembly techniques to connect the phenomena of nanoscience with the macroscale world in which we live, it will be possible to develop materials with novel capabilities, thereby leading to new tools and technologies. For example, a parallel Laboratory initiative is focused on developing an understanding of the operation and interaction of biological systems such as cells and proteins. These are the functional units of biology at the nanoscale and their decoding offers enormous potential not only for novel therapies but also for highly specific detectors and efficient, waste-free molecular factories. Achieving these applications, however, requires a concomitant materials technology to manipulate and interact with these units, thus translating their signals and returning instructions. If we do not learn to connect the nanoscale functional units of biology and chemistry to our conventional, macroscopic world, their true potential to revolutionize technology will not be realized.

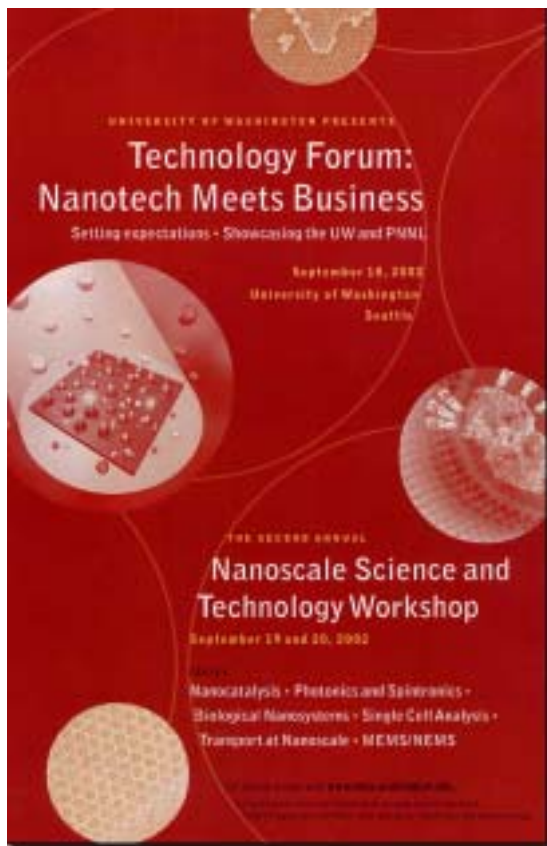
3.3.1 Research Strategy

The expected outcome of this initiative is a strong scientific foundation in nanoscience and technology upon which a range of Laboratory programs will be built, making Pacific Northwest National Laboratory a recognized leader in targeted areas of scientific inquiry at the nanoscale and application to DOE mission areas. Our strategy for developing this capability and reputation is to focus on selected areas that build on Laboratory strengths and to leverage these strengths by forming strategic alliances with regional universities and other national laboratories.

The challenge that must be met before moving forward from the scientific promise of nanoscience to the practical application of nanotechnology is twofold: 1) designing and manipulating molecular-scale structures, and 2) assembling these nanostructures into functioning systems capable of interfacing with the human scale world. The ability to direct self-assembly is imperative to convert the potential of nanoscience into the reality of nanotechnology. Nanoscience is further characterized by the importance of interfaces; the properties of nanoscale structures are by their nature dominated by surface and interfacial effects rather than bulk properties. Furthermore, the importance of molecular or biomolecular species at this length scale coupled with the aforementioned requirement to interface to the macroscale leads to a disciplinary interface between physics, biology, and chemistry, eventually encompassing electrical, mechanical, and chemical engineering.

We have successfully applied the Laboratory's existing strengths in metal oxide ceramics, oxide-organic and metal-organic interfaces to assemble novel meso- and nano-structured systems and developed a new modeling capability which allows us to understand the process of assembly. In the field of energy systems, we have modified known procedures for fabricating nanoporous silica and applied them to develop a low temperature process for fabricating photoconductive nanostructured titania. These structures, sensitized with a monolayer of organic dye, show promise for efficient, low cost solar cells but have never before been grown in a structurally controlled manner. Again, our focus is on assembled systems of nanoscale elements rather than the individual elements themselves. Other research

Nanoscience challenges us to visualize, synthesize, and manipulate structures that have dimensions on the order of the size of molecules and molecular clusters for a wide variety of technology applications.



The formation of the Joint Institute for Nanoscience with the University of Washington joins complementary expertise in nanomaterials and nanobiology and provides graduate-level educational opportunities for the next generation of technical leaders in nanoscience and nanotechnology.

projects have developed fundamental understanding of the assembly of metal oxide nanowire and quantum dot arrays for catalytic and detection applications. We also are building a core capability in dilute magnetic semiconductors where our unique materials, which retain their magnetic properties at well above room temperature, will allow the creation of systems to study the physics of spin polarized electron injection across semiconductor interfaces.

We will continue to develop depth in the above areas and initiate research into using similar structures to address problems in heterogeneous catalysis such as artificial photosynthesis for carbon reduction. Furthermore, we will use similar hierarchical structures to simulate and interface with nanobiological systems, thereby harnessing our new understanding of systems biology for mission applications.

In FY 2002 we successfully launched the Joint Institute for Nanoscience (JIN) fellowship program, which supports collaborative research with university students, postdoctoral associates, and faculty to work on relevant problems at the Laboratory. The JIN also encourages laboratory personnel to develop educational experience and together we have successfully obtained National Science Foundation funding to support joint nanoscience curriculum development between the university and the Laboratory. Our aim is to include other universities in the Pacific Northwest, creating a regional center to focus on nanoscience and nanotechnology. We will actively continue to seek sustainable external funding for the long-term future of an expanded nanoscience institute.

3.3.2 Topical Research Areas of Emphasis

Nano-catalysis: Nanostructures intrinsically maximize the surface to volume ratio of a material and as such are of intense interest to

the field of catalysis. However, the nanoscale may have catalytic implications beyond simply presenting a high surface area to one or more reactants. For example, the observation that small metal clusters exhibit lattice constants and surface energy states which differ from those found in the bulk material is consistent with a known impact on catalytic efficiency. At the nanoscale, the surface electronic structure and the transport of mass and charge become size-dependent, effectively allowing us to tune the chemical reactivity of the material. Research leading to new materials or materials systems with unique properties that cannot be realized on the macroscale are sought in this area, consistent with our focus on oxide materials and hierarchical, bottom-up assembly. Example projects include the controlled synthesis and catalytic properties of oxide quantum dots and nanowires, the former made using stress-controlled relaxation of epitaxial layers grown using PNNL's oxygen plasma assisted molecular beam epitaxy facility and the latter made using a novel, high angle ballistic deposition apparatus and the EMSL trace gas desorption analysis capability. Dramatic differences in binding sites and catalytic properties at the nanoscale have already been observed, as well as examples of enhanced stability, for example a material normally soluble in aqueous solution can be stable in quantum dot form. A modeling and simulation effort is highly focused and designed to directly support these experimental programs.

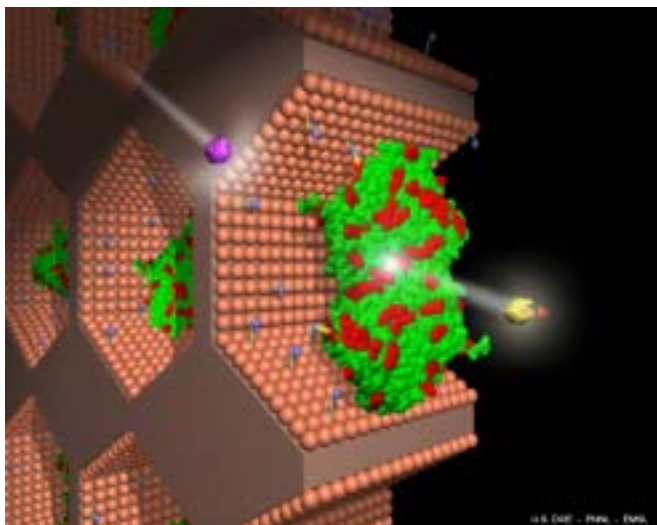
Nanostructural and Nanobiological Approaches to Preconcentration and

Detection: With particular relevance to Homeland Security, these individual areas fall naturally into one subject area at PNNL. The “holy grail” of detection is specificity—the ability to eliminate signals from extraneous sources—and there are no more specific interactions than those between enzymes and DNA interaction and between oligonucleotides, the nanobiological machinery of life. Many useful phenomena that occur at the interface between organic (including bio-organic) and inorganic materials remain poorly understood and therefore difficult to control. We have already made progress in understanding the synthesis and structure/property characteristics of such interfaces created by self-assembly or by other strategies. The combination of self-assembled systems with fabricated structures and the integration of the top-down approach (designed or engineered structures) with the bottom-up approach (systems that self-assemble) is likely to be an essential tool for many applications that seek to bridge the scale from the nano-size to the macro-size. Combination of these two processes (in soft materials interfaces and other areas described below) will enable integrated, functional systems to be created using nano-sized subunits. In particular, we are studying the problems of signal transduction from biological sensors and their stability in an immobilized matrix, the synthesis of surfaces that mimic enzyme action and using aligned arrays of multi-walled carbon nanotubes as preconcentrators for trace detection. Early results have already shown denaturing rates which are orders of magnitude lower for partially-encapsulated, single enzyme nanoparticles than for similar, unencapsulated enzymes in aqueous solution. Future work will study the immobilization of arrays of these bio-nanoparticles on porous, conductive supports for signal transduction.

Nanoscale Magnetic Semiconductors: PNNL has made significant progress in the development of a new dilute magnetic semiconductor based upon cobalt doped titania (anatase phase) grown epitaxially using oxygen plasma assisted molecular beam epitaxy. Pioneering work has shown that this material maintains strongly magnetic up to a Curie temperature of 700K, whereas the more widely studied materials based on III-V semiconductors are at best weakly magnetic at room temperature. This material, and the ability to controllably grow it at PNNL, therefore represents an enabling technology with which to investigate the basic physics of spin electronics and ultimately to enable practical applications.

Practical use of such a material, for example in magnetic memory applications, demands further fundamental research focused upon spin transport across interfaces, particularly when integrated with conventional silicon-based electronics. Both the structure and the chemistry of the interface control this process. Our research directions involve understanding how an interface interacts with the spin state of an electron and how an interface must be modified to minimize that interaction and thereby maintain the spin state of the carrier. Simulation of interfacial response to spin/charge transport, while necessary to guide interface design, nonetheless presents a challenge to the modeling community. We can presently simulate dielectric susceptibility variations with interfacial architecture and resident chemistry based upon local field codes developed in our “Thin Film Optical Materials” BES program. It is likely that the same codes could be modified to simulate the magnetic susceptibility of an engineered interface. Activities in this area are intended to modify existing local field codes to include magnetic properties.

The nanoscience and technology initiative is laying the foundation of scientific understanding that we hope will enable new research directions in our applied Directorates to solve practical problems such as NO_x reduction, hydrogen storage and photo-catalytic water splitting.



The anticipated range of applications for nanostructured materials or systems whose functional unit is nano-sized is immense. In each case, understanding and engineering the interface to the macro-world will be a critical factor in achieving functionality. The image above is an artist's conception of a cutaway view of an immobilized enzyme within a functionalized nanoporous silica pore. This environment stabilizes and increases the chemical reactivity of the enzyme, allowing it to convert harmful material into useful or harmless products.

The Laboratory has a strong commitment to support this activity both with internal funds and by providing support to develop new research proposals and industrial partnerships. A fundamental understanding of polarized spin transport at interfaces which leads to discovery of new materials systems has the possibility of revolutionizing MRAM (magnetic random access memory) applications that will promote development of fast and persistent memory in computers.

3.3.3 Link to the DOE Research Agenda

The Nanoscience and Nanotechnology initiative draws from existing Laboratory strengths in materials science and computation, and will build an expanded research and development agenda with application to all DOE core mission areas with our emphasis on nanoscale chemistry and detection, lending particular relevance to the Homeland Security mission. In particular, we aim to understand and exploit the nature of nanoscale systems and processes for

- understanding the adsorption of chemical moieties into nanoporous materials, including applications in catalysis, waste localization, and enzyme activity
- controlling charge transport in materials based on nanostructured arrays with the potential to improve the efficiency of renewable, point-of-use power generation to improve energy security
- understanding the growth and properties of novel magnetic nanostructures for high density information storage and secure communications
- combining engineered and self-assembled components into novel sensors for chemical and biological hazards to thwart bioterrorism
- accessing the properties of nanobiological systems such as enzymes and other proteins and anchoring them into porous oxide protein factories to develop new sensors and new green manufacturing routes.

The anticipated range of applications for nanostructured materials or systems whose functional unit is nano-sized is immense and, in each case, understanding and engineering the interface to the macro-world will be a critical factor in achieving functionality. One of the major objectives of the initiative is to facilitate the formation of the critical collaborations both between scientific disciplines and among basic and applied scientists to form an effective conduit for information flow between the needs of our applied mission areas and the development of capability in fundamental science. We recognize that the biggest potential of nanoscience is over the long-term and that the dream of intelligently functioning nanomachines is some years away. It is, however, critically important to lay the foundation of scientific knowledge now in order to ensure competitiveness of the United States in the forthcoming technological revolution in this area.

3.4 Bio-Based Products

This initiative is developing distinctive new capabilities that will establish Pacific Northwest National Laboratory as a significant contributor to DOE's energy resources mission to provide secure energy supplies. By enhancing our capabilities in the biological, chemical, and process sciences, we are developing new technologies to produce chemicals, materials, fuels, and power from renewable biomass resources instead of finite fossil resources, with processes that are more energy efficient and environmentally friendly than existing processes. This addresses several important national needs, including reducing the United States reliance on foreign petroleum, creating new markets for agriculture, and reducing environmental impacts.

The hallmark of our research has been development of processes that use novel heterogeneous catalysts to convert sugars and organic acids (dilute in an aqueous stream) to chemicals such as monomers for plastics, fibers, solvents, and adhesives. This initiative extends that existing capability to include discovery, screening, and manipulation of novel eukaryotic microorganisms for use in new fermentation processes (to produce organic acids, enzymes, and other products). In addition, the initiative will continue to enhance our nationally recognized condensed-phase catalysis capability and develop supporting process technologies (e.g., chromatographic and membrane separations, micro- and nanoscale technology) to reduce the capital and energy intensity of biomass conversion processes. The result of the initiative will be a portfolio of innovative processes that will provide financially attractive systems for the integrated "biorefinery" – a manufacturing system that simultaneously produces bioproducts, fuels, and power from biomass similar to the way a petroleum refinery produces an integrated suite of products from oil.

3.4.1 Research Strategy

The Laboratory is building upon our strong scientific base in chemistry, chemical engineering, applied microbiology, and growing capabilities in molecular biology to apply these to bioproducts research. This research leverages the Laboratory's distinct facilities and instrumentation, such as the state-of-the-art nuclear magnetic resonance and electron paramagnetic resonance instruments located in the Environmental Molecular Sciences Laboratory, and the advanced analytical and reactor equipment in the Chemical Engineering and Process Development laboratories. With this scientific base, we will continue to develop and advance systems to utilize the low-value biomass resources that are accumulated during normal production and processing of agricultural and forest products and cost-effectively convert those products into high-value chemicals, materials, fuels, and power.

Our research strategy will enable the resolution of several current barriers that preclude successful and cost-efficient conversion of biomass into energy and industrial products. For instance, coupled biological and catalytic conversion processes can provide significant technological and cost advantages over existing processing strategies. By using novel eukaryotic organisms to produce high yields of intermediate "platform chemicals," novel catalytic conversion routes can be used that significantly increase overall yield and reduce processing and energy

The emphasis of our bio-based products research is the development of integrated chemical and biological processes to produce high-value bioproducts such as commodity and specialty chemicals.

costs. Advanced catalytic conversion/synthesis technologies also provide the opportunity to produce entirely new materials by utilizing compounds and chemical structures unique to biomass.

Pacific Northwest National Laboratory investments are concentrated in three primary research areas:

- **Heterogeneous catalysis.** One of the key technical hurdles associated with catalysis processes has been the need to develop catalyst systems that afford high selectivity to the desired products, while minimizing mass transfer limitations and maintaining performance over long periods of operation. A particular limitation has been the need for catalyst support materials that possess the appropriate functionality for the reactions of interest. Through this initiative, we are developing a fundamental understanding of the relationship between support system modification and catalyst performance. This will significantly enhance our overall catalyst synthesis and characterization capability, and provide the basis for developing robust catalyst formulations for high-activity, high-specificity hydrogenation, hydrogenolysis, and oxidation reactions.
- **Eukaryotic organisms in fermentation and enzyme discovery.** The Laboratory has a group dedicated to fully exploring and exploiting the characteristics and capabilities of filamentous fungi, the class of microorganisms largely responsible for recycling lignocellulosic biomass in nature and the source of beta lactam antibiotics (miracle drugs of the 20th century). These eukaryotic organisms have been largely ignored for development of new fermentation systems and enzyme discovery. Only a few of the hundreds of thousands of known fungal species are currently in use for manufacture of useful products via large-scale culture. These organisms are less well studied and are generally less exploited than other groups of microbes. The Laboratory has established the ability to study and manipulate these organisms by building a culture collection for discovery, characterization, and product screening; establishing a fermentation laboratory; and developing novel molecular biology tools for genetic manipulation of the fungi as part of developing optimal production systems.



Pacific Northwest National Laboratory signed a memorandum of understanding with the Idaho National Engineering and Environmental Laboratory, Washington State University, and the University of Idaho to form the Northwest Bioproducts Research Institute, a regional center of excellence for bio-based products research and development.

- **Separations and other supporting process technology.** An integrated suite of separations and process technology is needed to optimally and efficiently convert biomass into energy and industrial products. Understanding how various processing steps affect one another is critical to the overall success of an integrated “biorefinery” and necessary for rapidly translating scientific discoveries into deployable technologies. Advanced, integrated systems are also needed to reduce the capital and energy intensity of new processes. Our core capabilities in chemical process science and technology, and analytical chemistry will be used and enhanced to develop novel approaches to feedstock pretreatment, conversion, and product purification. Our focus is on ensuring effective recovery of value from all biomass fractions (including proteins, lipids, and fiber, and carbohydrates) in an energy-efficient manner. We also will develop novel reactor and separation systems, such as advanced microthermal and chemical systems, to provide the process intensification necessary to significantly reduce the capital and energy requirements for biomass conversion and separation.

3.4.2 Role in the DOE Research Agenda

This research directly supports the President’s National Energy Plan and the Department of Energy’s energy resources mission. Research on novel processes to convert biomass to products, fuels, and power is a core element of the Office of Energy Efficiency and Renewable Energy’s research portfolio, and will result several positive benefits including reducing the nation’s dependence on foreign oil. We expect to draw heavily on the Office of Science supported capabilities in fundamental life sciences research to enable this agenda.

3.5 Carbon Management

Carbon management is the science, technology, and policy required for the world to stabilize the atmospheric concentration of greenhouse gases at a level that minimizes adverse impacts on the environment, as well as human and economic systems.

This initiative will

- further our basic understanding of the science, technology, and policy required to stabilize atmospheric carbon. This knowledge will enable Pacific Northwest National Laboratory to be instrumental in shaping the Department of Energy’s and the nation’s efforts to develop carbon management solutions. To accomplish this, we will expand our understanding of the economic, environmental, and social dimensions of technological and natural systems. Particular emphasis will be placed on energy systems and their relationship to the earth’s natural systems.
- conduct basic research on specific carbon management technologies (such as low-carbon fuels, bioenergy, and carbon sequestration technologies) that are novel and that are identified as critical to solving the climate change problem.

Progress toward these goals includes the following:

To advance our basic understanding of the science, technology, and policy required to stabilize atmospheric carbon, the Laboratory is investing resources in technology and economic modeling concepts that will provide the essential foundation for **next generation integrated assessment models**. Integrated assessment models combine computational representations of atmospheric systems, oceans systems, agricultural systems, energy systems, and economic systems, thereby enabling scientists, and ultimately policymakers, to better understand the complex interrelationships that are associated with the world in which we live. This improved understanding will make it possible to develop climate change response strategies that effectively address climate change, while minimizing any negative economic, social, or environmental side effects.

In collaboration with the University of Maryland, we established the **Joint Global Change Research Institute**. The work of this Institute will contribute to the understanding of the science, economics, and technology of energy and the environment, connecting its work to the national and international policy communities, and developing educational opportunities to train university students in these areas. The Institute will operate programs in the following areas of research: integrated assessment modeling, technology strategies to address climate change, resource modeling and assessment, vulnerability and adaptation studies, local and global environmental mitigation

Pacific Northwest National Laboratory and the National Energy Technology Laboratory will expand their joint analytical efforts on sequestration and carbon management – the nation’s largest individual sequestration project.

measures, and dialogues around global change issues across disciplines and national boundaries and among diverse socioeconomic stakeholders.

We also made major progress expanding our research base in **soil carbon sequestration** and began defining a science and technology thrust in engineered carbon capture and sequestration. In 2002, Pacific Northwest National Laboratory began work on public-private program with DOE Office of Fossil Energy's National Energy Technology Laboratory that will explore the suitability of deep geologic formations for carbon sequestration. These actions support our goal of conducting basic research on specific carbon management technologies (such as low-carbon fuels, bioenergy, and carbon sequestration technologies) that are novel and that are identified as critical to solving the climate change problem.

In the area of soil carbon sequestration, the Laboratory helped establish the **Consortium for Agricultural Soils Mitigation of Greenhouse Gases**,

which will be initially funded by the U.S. Department of Agriculture at \$15 million total for fiscal years 2001 and 2002. The goal of this consortium is to provide the scientific tools and information needed to successfully implement soil carbon sequestration and greenhouse gas reduction programs so that we may lower the accumulation of greenhouse gases in the atmosphere while providing income and incentives to farmers and improving the soil. The consortium brings together the nation's top researchers in the areas of soil carbon, greenhouse gas emissions, conservation practices, computer modeling, and economic analysis to accomplish the goal. Specific activities that will be conducted in pursuit of the goal include basic research on processes and mechanisms of soil carbon sequestration, development and assessment of best management practices, prediction and assessment of



Pacific Northwest National Laboratory's Carbon Management initiative strives to further understand the science, technology, and policy required to stabilize atmospheric carbon.

carbon sequestration and greenhouse gas emissions, measurement and monitoring of greenhouse gas emissions and emission reductions, outreach, and technology transfer.

Our role in this consortium complements our basic science role in the DOE-funded **Center for Carbon Sequestration in Terrestrial Ecosystems (C-SITE)**. DOE's Office of Science, following the scientific peer review process, extended the Laboratory's role in C-SITE for another 3 years. This role provides leadership opportunities for the Laboratory in the nation's two premier programs that address soil carbon sequestration.

3.5.1 Research Strategy

Most national and international efforts to identify climate change solutions focus on the near-term actions that are needed to reduce carbon emissions. While significant near-term actions are required, climate change is a global, century-scale

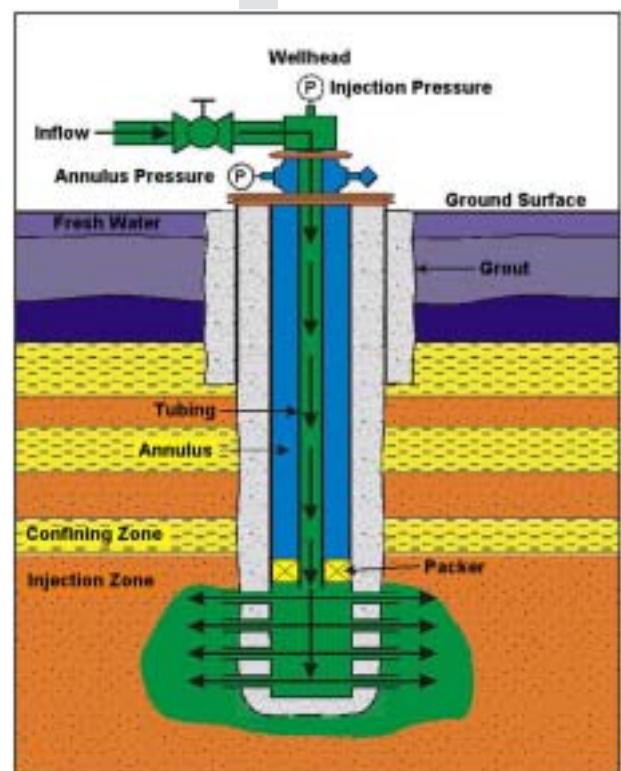
problem. We believe that it must be solved with a global, century-scale carbon management approach, and near-term actions must be taken within the context of this century-scale strategy.

Over a diverse range of scenarios, future carbon emissions are estimated to be considerably higher than the allowable level of emissions that would ultimately lead to stabilization of atmospheric greenhouse gas concentrations. Developing and deploying the low-carbon technologies that will enable us to close the “gap” between expected future emissions and a level of future emissions that will enable stabilization of atmospheric greenhouse gas concentrations is a monumental challenge.

Addressing this challenge requires a contribution from three major science and technology domains: 1) climate science, which enables a fundamental scientific understanding of the problem; 2) integrated assessment, which enables the formulation of carbon management strategies and systematic evaluation of trade-offs and uncertainties; and 3) energy technology development. Pacific Northwest National Laboratory’s institutional strategy is to ensure that the Laboratory’s programs in each of these areas are technically integrated across the Laboratory, such that new discoveries in climate change science are rapidly factored into carbon management strategies. In addition, given the complexity of each of these domains, the Laboratory’s strategy is to engage and rely upon the broader scientific and industrial communities to complement our internal capabilities.

Within these three domains, capability development investments supported by this initiative will be focused in two key areas:

- Integrated Assessment.** We will provide intellectual leadership across the DOE complex with respect to an integrated carbon management approach. This activity will be a logical extension of our current work and will be an area where the Laboratory is viewed by DOE, industry, and the scientific community as working at the leading edge of science. Specific near-term efforts will focus on advanced computational approaches for modeling technological, economic, agricultural, and earth systems in an integrated fashion to develop a higher level of understanding between the components of earth and natural systems. We also will explore approaches for extending to global scales the analysis of climate change impacts on managed ecosystems through use of simulation models, geographic information systems, and global datasets. Our aspiration also is to move this modeling capability toward computational architecture that enables collaborative problem solving. These scientific goals will directly support the stated goals of the President’s National Climate Change Technology Initiative and Climate Change Research Initiative.
- Carbon Sequestration.** Our research on carbon sequestration will address engineered carbon capture from industrial and utility sector flue gases coupled with CO₂ disposal in deep geologic formations. Although there are



Pacific Northwest National Laboratory scientists are studying the flow and chemical reaction processes of CO₂ at high pressure in basalt and sedimentary rock formations to assess the potential of these formations to permanently sequester CO₂.

many types of geologic sequestration, we will focus on three: CO₂ sequestration in deep, brine-filled sedimentary formations; CO₂ sequestration through in situ mineralization; and simultaneous production of methane hydrates and CO₂ sequestration. The Laboratory's existing capabilities in geochemistry, reactive transport modeling, spectroscopy, and fluid dynamics will all be extended and applied to this new scientific area. Further, to assist in deployment of the science to practical problems, we will continue to extend our growing list of industrial collaborators.

3.5.2 Role in the DOE Research Agenda

The Carbon Management initiative is directly aligned with two DOE missions: science and energy resources. The Office of Science recognizes the integrated assessment, understanding of the carbon cycle, and terrestrial sequestration as increasingly important components of its missions. The Office of Fossil Energy has primary mission responsibility for geologic sequestration.

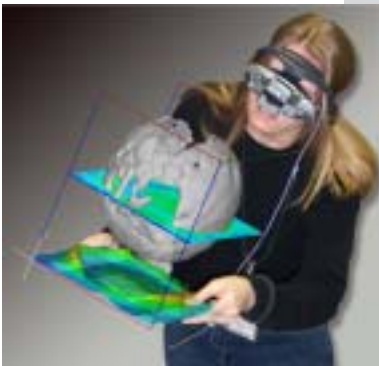
3.6 Imaging Science and Technology

Image analysts and investigators in many different applications face common challenges in processing an overwhelming amount of increasingly complex image data. In addition, they must deal with many complex software analysis packages, each of which provides only a partial solution. Pacific Northwest National Laboratory is responding to these needs through this initiative by developing new image processing algorithms, image fusion methodologies, and three-dimensional data visualization tools for multiple domain applications. Applications receiving specific focus are remote sensing of the earth for national security and natural resource management missions, cell imaging for systems biology investigations, and ultrasonic imaging of engineered materials for energy applications. Ultimately, the goal of the initiative is to enable end-users to gain greater value and insight from image-assisted investigations, to improve the productivity and accuracy of image analysis, and to bring about more effective data interpretations and decision outcomes.

3.6.1 Research Strategy

To achieve these goals, this initiative is pursuing a multielement phased strategy. During the first phase of the initiative (through mid-fiscal year 2002), the focus will be on developing algorithms and methods that are broadly applicable to many end-use applications, and includes the following four elements:

- Develop a suite of mathematical algorithms and flexible software tools for analysis of multisensor imagery. Research and development is focused on overcoming major challenges in image registration, automated feature extraction, and multi-image fusion.
- Develop three-dimensional image visualization and interaction tools that increase the ability of humans to understand, interpret, and make decisions based on multisensor image data.



Imagery visualization and interaction tools are being developed to accelerate the rate of scientific understanding of complex biological phenomena.

- Build on the Laboratory's strengths and ongoing investments in parallel, distributed computing. The algorithms developed under this initiative are being imported into a software architecture and parallel computing environment being funded by the Computational Science and Engineering initiative as a joint effort.
- Create a flexible and extensible software architecture for integrating image analysis algorithms and visualization tools that will enable researchers across multiple disciplines to easily share, adapt, and evaluate analysis methods, algorithms, and visualization tools.

In order to mature the most promising methods and technologies further, it is necessary to focus them on specific applications. Consequently, efforts during the second half of fiscal years 2002 and 2003 consist of two elements:

- Shift the development activities into an environment where multiple tools (e.g., registration, feature extraction, visualization) can be codeveloped, integrated, and applied to specific problems in remote sensing, cell imaging and materials characterization. The resulting problem solution components will be merged with commercial and open-source software tools, to create a useful, prototype, imaging analysis tool suite.
- Shift the research focus to the challenging and important requirements posed by very high-dimensionality imagery data, i.e., data having two (pixels) or three (voxels) spatial dimensions, coupled with high levels of temporal or spectral complexity.

3.6.2 Research Areas of Emphasis

Research activities are focused on the following areas:

- **Image registration**, including image-to-image registration, geo-registration and model-to-image fusion. Two novel techniques for image registration have been developed and investigated: Comparative Information Theory and Geometrically Invariant Parameter Space Clustering (GIPSC). Development and extension of the GIPSC methodology will continue in fiscal year 2003.
- **Feature extraction and change detection**. In fiscal years 2001 and 2002, new methods were developed that provided improved image-to-image resolution, interpolation, change detection, and fusion of different image types such as optical and magnetic resonance images. In fiscal year 2003, emphasis will be placed on the development of statistical methods for automatically identifying features and segmenting images, which is based on a different approach for statistically analyzing the spatial characteristics of images.
- **Image and information fusion methods** have been developed for bringing three-dimensional, computer-generated models of buildings into a visualization and analysis environment. This capability is critical to the creation of well-characterized three-dimensional models that are then coupled with imagery and infrared atmospheric measurements to characterize chemical effluents coming from sites suspected of producing nuclear, chemical, or biological weapons. Work in this area will be continued under a new program funded by the Office of Nuclear Nonproliferation (NA-22).



Statistical feature extraction and classifications have been developed to group segments of a satellite image of the Hanford area (top image) into clusters having similar characteristics such as farmland, river, or native terrain.

- **Imagery visualization and software integration.** An expanded imagery visualization and interaction capability has been developed and is embodied in the Human Interaction Workspace or “HI-SPACE” visualization system. This system portrays imagery in a three-dimensional, augmented reality environment that enables researchers to visualize and interact with their data. The underlying concepts for an integrating architecture is also being developed that will enable researchers and analysts to more readily share data and analysis tools across disciplines and computing platforms.

These general areas of research will continue into fiscal year 2003 with increased focus on the very difficult scientific challenges imposed by high-dimensionality imagery, i.e., where combinations of three or more spatial and time dimensions, and multiple spectral bands, must all be simultaneously analyzed.

3.6.3 Role in the DOE Research Agenda

This initiative directly contributes to the following Department of Energy mission areas:

- In National Security, digital imaging processing algorithms are providing analysts the ability to more rapidly and effectively register, fuse, and exploit multisensor imagery. Tools are being developed to combine imagery consisting of multiple spectral bands and sensor types, and then integrating this imagery with three-dimensional site models and atmospheric chemical measurements. This synthesis creates a more complete signature and assessment of the true nature of the suspected activities, such as from a chemical weapon production facility. The resulting capabilities and tools are directly relevant to DOE’s missions in nonproliferation and counterterrorism.
- The imaging technology under development has direct applications to DOE’s science mission in the areas of visualization of molecular, cellular, and tissue structures, and to dynamic biological processes. The algorithms and tools coming from this initiative are being specifically focused on the unique data being produced by the instruments in Pacific Northwest National Laboratory’s Cellular Observatory. The development of methods for registering and extracting features from fused image data obtained by several modalities (e.g., confocal microscopy, nuclear magnetic resonance, and correlated anti-Stokes Raman spectroscopy) is also an active area of investigation.
- In the mission area of Environmental Quality, image processing and analysis tools are being developed that improve the interpretation of ground, aerial, or space photography for surveillance of waste sites, land use and restoration, and management of disaster events. Assessment tools resulting from this initiative support DOE’s Global Climate Change Program by more effective identification of potential sites of underground sequestration of carbon dioxide. Methods resulting from this initiative will enable analysts to enhance the spatial and spectral information that can be obtained from lower-cost, lower-resolution imagery. Since environmental applications often involve characterization of very large tracts of land, these tools will provide a higher level of information while reducing overall imaging costs.
- Imaging analysis methods are improving the efficiency of locating and characterizing potential fossil energy sources and sites for underground sequestration of carbon dioxide, which supports DOE’s mission in Energy

Resources. These methods will also enhance the characterization of transportation corridors and power lines and location of energy generation facilities. Regarding materials characterization applications, work currently under way in the initiative supports DOE's interests in nuclear plant aging and life extension and can be extended to address materials characterization needs in other materials-intensive areas such as advanced fuel cells.

3.7 Energy Systems Transformation

Strong economic growth in the last decade, coupled with new economic forces unleashed by energy deregulation, has stressed our energy system. Power reliability has degraded. Market distortions have created volatile prices with significantly increased costs to consumers and added risk on needed investments in generation and transmission. In implementing the President's National Energy Strategy, the focus has been on ensuring that initiatives are undertaken that fundamentally revolutionize the ways we produce and consume energy rather than promoting incremental change.

A fundamental transformation of our generation, transmission, distribution, and end-use energy systems must occur for the Department of Energy to reach these goals. No single energy technology is on the horizon to spawn this transformation. A systems view, leveraging information technology that has yet to impact energy systems as it has other sectors, is required. To make deregulated energy markets function effectively and to integrate new distributed energy technologies, clear economic signals combined with power and performance data must be used by all parts of the system to create collaborative opportunities for reducing costs and increasing asset utilization and efficiency. This is now possible because of advances in information and telecommunications technology. These advancements facilitate the creation of distributed management and control solutions that transfer price, supply, and demand signals across enhanced energy networks, effectively eliminating market distortions.

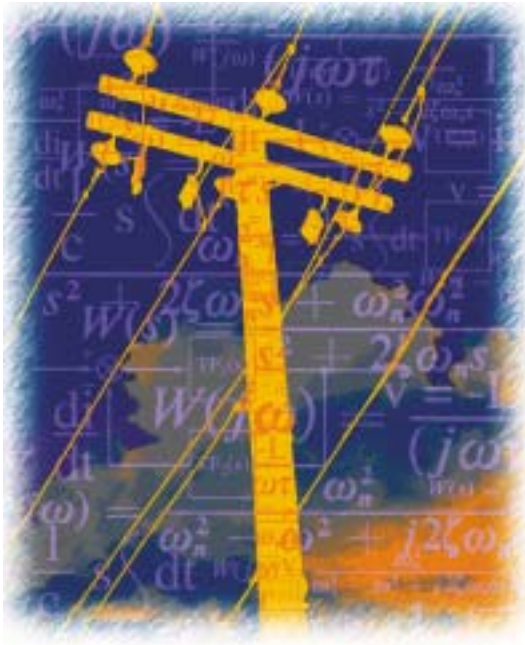
The goal of the Energy Systems Transformation initiative is to research, develop, and deploy a new generation of energy networks. The advent of distributed and embedded digital intelligence in virtually all devices, at low cost, offers the opportunity to fundamentally change our energy systems. This transformation will allow a much more flexible system control and more efficient matching of loads with electricity and gas supply through coordinated end-use management and remote, energy-resource dispatching. Enabling remote resources to interact with the system will facilitate the use of distributed generation, a key requirement for the incorporation of renewable energy sources and high-efficiency combined cycle systems.

3.7.1 Research Strategy

The Energy Systems Transformation initiative is providing a central role for the Laboratory in a new national program that will develop the tools, technologies, policies, and market mechanisms to deliver significant increases in the overall performance of the nation's energy systems. We will explore the impacts of new technologies on the energy system such as wind, photovoltaics, fuel cells, micro-turbines, storage, and energy efficiency. Realizing the advantages of a transformed

The President's National Energy Strategy summarizes the broad challenge we face as a nation – to ensure that the massive infrastructure investments required for new central power plants, transmission, and distribution are balanced with end-use efficiency, distributed generation, and renewable energy to create a cleaner, cheaper, and more reliable energy system.

energy system requires breakthroughs in the level of understanding of the complex interactive nature of the system and markets and how various resources can best be deployed.



Our focus in the Energy Systems Transformation initiative is on state-of-the-art mathematical models, economics, and computations to create a next-generation system simulation.

Historically, energy systems have been constructed and operated independently, with little communication across boundaries, other than one-way transfer of commodity and billing (a downward transfer), and metered usage and payments (an upward transfer) through the physical and financial networks, respectively. The control of these systems is almost entirely void of any shared information or planning processes and is heavily dependent upon human operators. Our goal is to create an information-rich energy network that will enable more complex market transactions and more complex system control and operation, enhancing opportunities for collaboration. This creates a myriad of technology opportunities to develop software and hardware applications, such as grid-friendly appliances, financial transactions and market operations, new process controls for grid operations and distributed generation, load forecasting and management tools, and diagnostics and prognostics.

3.7.2 Research Areas of Emphasis

Research activities in fiscal year 2002 are focused on developing 1) an agent-based simulation, combining markets, supply, grid, and dynamic distribution system loads; and 2) decision-network analysis techniques for dynamic control and optimization of the co-joined economic and engineering systems. The long-term intent is to accurately predict the

impacts and benefits of dynamic, adaptive markets and new technologies to inform policy, analyze technology options, understand market dynamics, and create operational strategies. Industry's involvement is critical to guide and target our efforts. Through a series of workshops, this initiative has begun to catalyze a new public/private partnership to design, develop, and deploy these new networks and systems. As a result, the Laboratory is leading a new DOE program on Advanced Communication and Control for Distributed Energy System Operations focused on

- a system architecture of communication networks and information protocols required for integrating financial, control, planning, and operations networks while ensuring security, privacy, and reliability
- a variety of pilot projects, laboratory experiments, and field tests to provide a rigorous validation of the simulation, the networks, and the applications through a range of conditions and locations.

3.7.3 Role in the DOE Research Agenda

The Energy Systems Transformation initiative is directly aligned with the missions of the Office of Energy Efficiency and Renewable Energy and the Office of Fossil Energy to develop and deploy efficient, clean, and reliable energy resources. Our application of fundamental mathematical modeling and computer science capabilities strongly aligns with similar efforts in the Office of Science. The transformed energy system can have important positive impact on national security by increasing the distributed nature and self-healing properties of our energy

systems and by supporting a broad spectrum of crisis management strategies and tactics. We also are working closely with the Bonneville Power Administration and others to validate and field test applications and to position the region as a center for expertise and technology.

3.8 Advanced Nuclear Science and Technology

The vision of the Advanced Nuclear Science and Technology initiative is to assess, refocus, and reinvigorate business and technical capabilities in nuclear science and technology at Pacific Northwest National Laboratory to enable leadership and program growth in strategic mission areas.

Pacific Northwest National Laboratory has provided nuclear science and technology to support DOE's energy, environmental, and national security missions since 1965. A strong nuclear science and technology capability at the Laboratory will make major and positive contributions to the Laboratory signature, Department of Energy core mission needs, and critical global energy needs. Important issues must be addressed and resolved if the Laboratory is to maintain and potentially grow its nuclear science and technology-based programs and business. Key Laboratory capabilities, technologies, and facilities in nuclear science and technology must be developed, maintained, and strengthened.



Applying nearly 40 years of material science and reactor expertise, Pacific Northwest National Laboratory is working with the nuclear industry to extend the life of existing reactors and developing new advanced reactor designs.

3.8.1 Research Strategy and Areas of Emphasis

The Advanced Nuclear Science and Technology initiative work in fiscal year 2002 focused on development of a strategic roadmap for the initiative that will establish the basis for Laboratory Directed Research and Development investments in fiscal years 2003 and 2004 and serve to position the Laboratory for program growth in five market-directed focus areas:

- Nuclear Energy, as part of a wider activity in Advanced Energy Technologies
- Nuclear Legacies, in particular address Hanford Site needs
- Homeland Security and National Defense
- Defense Nuclear Nonproliferation, in particular international programs
- Radiobiology, and other isotope applications.

3.8.2 Role in DOE Research Agenda

Our Advanced Nuclear Science and Technology Initiative (ANSTI) supports the goals of the Office of Nuclear Energy, Science and Technology aimed at promoting research and development to advance applications of nuclear technologies that improve U.S. energy security, economic vitality, and quality of life. Our alignment with this strategy includes:

- Applying and enhancing capabilities focused on building new nuclear power plants that can play an important role in the nation’s long-term energy security and provide clean, affordable alternatives to carbon emitting power plants.
- Developing diagnostic and prognostic tools to extend the productive lifetime of existing power plants.
- Pursuing advancements in medical isotope production.

The initiative also will align with the DOE research agenda by providing support to:

- The Office of Environmental Management and its accelerated cleanup mission at Hanford and other legacy sites, by striving to reduce programmatic risk, address technical uncertainties and provide science and technology solutions for decommissioning and decontamination projects.
- The Office of Basic Energy Sciences, in research missions that focus on the chemical and physical properties of materials behavior.
- Science and technology advancements related to sensing and detecting nuclear materials non-proliferation and attribution.
- Test and measurement to support National Nuclear Security Administration programmatic needs.

Table 3.1. Projected Sales Resulting From Laboratory Initiatives^(a)
(\$ in Millions)

Initiative	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Biomolecular Systems							
Office of Science							
Biological and Environmental Research	8.2	12.4	15.3	17.6	21.5	24.2	31.0
Advanced Scientific Computing Research	0.7	0.7	0.8	0.9	1.4	1.4	1.4
Basic Energy Sciences	0.5	0.3	0.3	0.3	0.3	0.3	0.3
Nonproliferation and National Security	0.6	0.7	1.0	1.0	1.0	1.0	1.1
Energy Efficiency and Renewable Energy	0.1	0.2	0.3	0.5	0.5	0.5	0.6
National Institutes of Health 1830	0.3	0.3	1.0	2.7	5.5	7.9	9.9
National Institutes of Health 1831		4.9	6.0	5.5	4.3	2.3	1.3
Office of Science Capital Equipment	3.6	1.1	1.5	1.9	1.8	1.5	
Total Biomolecular Systems	13.9	20.6	26.2	30.4	36.3	39.1	45.6
Computational Sciences and Engineering							
Office of Environmental Management	1.0	1.6	1.5	1.5	1.5	1.5	1.5
Office of Science							
Biological and Environmental Research	2.9	11.9	12.1	13.0	13.7	14.4	15.2
Advanced Scientific Computing Research	2.1	2.8	3.0	4.0	4.6	5.0	6.0
Basic Energy Sciences	0.4	1.2	1.7	1.7	2.0	2.2	2.3
Energy Efficiency and Fossil Energy	2.6	2.7	2.9	3.3	3.6	3.9	4.2

Table 3.1. Projected Sales Resulting From Laboratory Initiatives^(a) (contd)
(\$ in Millions)

Initiative	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Nonproliferation and National Security	0.3	0.3	0.7	1.5	2.0	2.0	2.0
Department of Defense	0.3	0.6	0.9	1.2	1.7	1.9	2.4
Other Federal Agencies	0.5	1.3	1.4	1.6	1.8	1.8	1.8
Office of Science Capital							
Advanced Scientific Computing Research	0.4	0.2	0.0	0.5	1.0	1.0	1.0
Total Computational Sciences and Engineering	10.5	22.6	24.2	28.3	31.9	33.7	36.4
Carbon Management							
Office of Science							
Biological and Environmental Research	1.0	1.7	2.5	3.0	3.0	3.0	3.0
Energy Efficiency (EE)		0.1	1.0	1.5	1.5	1.5	1.5
Fossil Energy (FE)	0.3	0.8	1.0	1.5	4	4	5.5
Environmental Protect Agency		0.3	0.3	0.5	0.5	0.5	0.5
Other Federal Agencies			1.0	2.0	2.0	2.0	2.0
Total Carbon Management	1.3	2.8	5.8	8.5	11.0	11.0	12.5
Nanoscience and Nanotechnology							
Office of Science							
Basic Energy Sciences	0.0	0.8	2.2	5.1	5.3	5.5	5.0
Biological and Environmental Research			0.8	1.2	1.6	1.9	2.2
Envir. Restoration and Waste Mgt. (EM)		0.4			0.2	0.3	0.4
Nonproliferation and National Security	0.0	0.1	0.1				
Department of Defense	0.0	0.7	0.9	1.1	1.3	1.5	1.7
Human Health Services/National Institutes of Health 1830	0.0	0.0	0.5	1	1.5	1.5	2
Human Health Services/National Institutes of Health 1831							
Other Federal Agencies	0.0	0.0	0.3	0.6	0.9	1.2	1.5
Total Nanoscience and Nanotechnology	0.0	2.0	4.8	9.0	10.8	11.9	12.9
Imaging Science and Technology							
Nonproliferation and National Security		0.2	1.9	3.3	3.5	3.5	3.5
Office of Intelligence (IN)	0.1	0.2	0.2	0.2	0.2	0.2	0.3
Fossil Energy	0.3	0.6	0.6	0.6	0.7	0.7	0.7
Office of Science							
Biological and Environmental Research			0.3	0.3	0.5	0.5	0.5
Basic Energy Sciences			0.2	0.4	0.5	0.5	0.5
Intelligence Community/Imaging and Mapping	0.2	0.5	0.5	0.8	2.0	2.7	2.7
Department of Defense	--	0.2	0.2	0.4	0.7	0.7	1.0
National Aeronautics and Space Administration	--	0.1	0.2	0.4	0.5	0.5	0.7
Human Health Services/National Institutes of Health 1830							
Human Health Services/National Institutes of Health 1831	--	0.2	0.5	1.0	1.2	1.5	2.0
Other Federal Agencies	--	--	0.1	0.3	0.5	0.5	0.5
Total Imaging Science and Technology	0.6	2.0	4.7	7.7	10.3	11.3	12.4

Table 3.1. Projected Sales Resulting From Laboratory Initiatives^(a) (contd)
 (\$ in Millions)

Initiative	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Bio-Based Products							
Office of Science							
Basic Energy Sciences				0.5	0.5	0.5	0.5
National Nuclear Security Administration				0.5	0.5	0.5	0.5
Energy Efficiency and Renewable Energy	1.0	2.0	5.9	6.9	8.8	10.6	10.5
Other Federal Agencies			0.1	0.1	0.25	0.4	0.5
Total Bio-Based Products	1.0	2.0	6.0	8.0	10.0	12.0	12.0
Advanced Nuclear Science and Technology							
Office of Environmental Management				0.25	0.5	1	1.2
Office of Science							
Basic Energy Sciences			0.2	0.5	0.7	0.9	1
National Nuclear Security Administration				0.1	0.3	0.5	0.7
Office of Nuclear Energy, Science, and Technology		0.4	1.7	2.0	3.0	3.6	4.4
Department of Defense				0.2	0.3	0.5	0.7
Nuclear Regulatory Commission			0.1	0.5	1.7	2.0	2.5
Office of Civilian Radioactive Waste Management		0.2	1.3	2.0	2.5	1.0	1.0
Other Federal Agencies			0.2	0.5	0.8	1.0	1.0
Total Advanced Nuclear Science and Technology	0.0	0.6	3.5	6.1	9.8	10.5	12.5
Energy Systems Transformation							
Office of Science							
Advanced Scientific Computing Research			0.2	0.5	0.5	1	3.5
Basic Energy Sciences				0.3	0.3	0.3	0.3
Energy Efficiency and Renewable Energy	0.0	2.3	2.5	4.0	5.0	6.0	8.0
Department of Defense				0.3	0.4	0.8	1.0
Other Federal Agencies	0.0		0.2	0.2	0.4	0.5	0.6
Total Energy Systems Transformation	0.0	2.3	2.7	4.5	5.8	7.3	9.6
Homeland Security							
Office of Science							
Biological and Environmental Research				0.3	0.5	0.5	0.5
Advanced Scientific Computing Research			0.3	0.5	1.2	1.5	1.5
Basic Energy Sciences				0.3	0.4	0.5	0.5
National Nuclear Security Administration				0.2	0.4	0.5	0.5
Other Department of Energy				0.1	0.1	0.1	0.1
Department of Defense			1.7	2.5	4.0	6.0	7.0
Other Federal Agencies - 1830			2.0	5.0	7.2	10.0	12.0
Other Federal Agencies - 1831							
State and Local Governments - 1831							
Industrial - 1831							
Total Homeland Security	0.0	0.0	4.0	8.9	13.8	19.1	22.1
Total Pacific Northwest National Laboratory Initiatives	27.3	54.8	81.8	111.3	139.7	155.9	176.0

(a) Initiatives are provided for consideration by the Department of Energy. Inclusion in this Plan does not imply DOE approval of or intent to implement an initiative.

4

Programmatic Strategy

4.1 Science

The U.S. Department of Energy's Pacific Northwest National Laboratory advances scientific discovery in the environmental, biological, computational and energy sciences. We advance the fundamental understanding of complex systems from the molecular to the global scale by building multi-disciplinary, multi-institutional teams across the physical, chemical, computational and biological sciences. We develop unique instrumentation that is the hallmark of the Laboratory's national user facilities.

4.1.1 Strategic Intent

Pacific Northwest National Laboratory strives to sustain existing strengths and develop new capabilities in its science base to address DOE's mission needs. Over the next 5 years, we will

- sustain and grow our strengths in biology and biogeochemistry, atmospheric science and global environmental change, materials and chemical sciences, and computational sciences
- provide effective stewardship of our scientific user facilities, particularly the William R. Wiley Environmental Molecular Sciences Laboratory
- establish our scientific leadership in systems biology with particular emphases on high-throughput proteomics, microbial systems, cell signaling, cell imaging, structural biology, and computational biology
- develop new expertise and capabilities in nanocatalysis and nanobiology based on existing resources in the Environmental Molecular Sciences Laboratory and new resources established in response to DOE mission needs
- seek new capabilities and resources to support research in systems biology consistent with the May 2002 Genomes to Life "DOE Resources and Technology Centers for Biological Discovery in the 21st Century" report
- develop leading capabilities in computational and simulation sciences and establish new key resources for computational biology, subsurface modeling and regional climate modeling based on a core expertise in computer science and applied mathematics
- provide scientific and programmatic leadership in climate, carbon sequestration, and aerosol research.

4.1.2 Our Role in the DOE Mission Portfolio

Research at Pacific Northwest National Laboratory provides the scientific tools and knowledge to support mission needs of the Office of Science by focusing on

the following areas: biology and biogeochemistry, atmospheric science and global environmental change, materials and chemical sciences, and computational science (see Table 4.1).

Table 4.1. Science Program Crosswalk		
Science Focuses	DOE Programs	B&R Codes
Biology and Biogeochemistry	Engineering and Geosciences; Energy Biosciences; Life Sciences; Environmental Remediation	KC-04, KC-06, KP-11, KP-13
Atmospheric Science and Global Environmental Change	Environmental Processes	KP-12
Materials and Chemical Sciences	Materials Sciences; Chemical Sciences, Engineering and Geosciences	KC-02, KC-03, KC-04
Computational Sciences	Mathematical, Information, and Computational	KJ-01

Microorganisms are increasingly recognized as dominant catalysts in the dissolution and precipitation of minerals and, as a result, the field of geomicrobiology is experiencing a renaissance.

4.1.2.1 Biology and Biogeochemistry

We provide innovative approaches for preventing the deleterious effects of energy use, mitigating its injurious outcomes, and protecting our environment, both now and in the future. The Laboratory’s international reputation in environmental microbiology and biogeochemistry, along with our premier capabilities in proteomics, mass spectrometry, cell imaging, and nuclear magnetic resonance spectrometry, provide the intellectual and technical foundation for new approaches to biology. On this foundation we are building a systems biology program focused on understanding energy and carbon flow in microbial communities and how cells respond to environmental stress. Our research in microbiology has direct application to producing clean energy, removing excess carbon dioxide from the atmosphere, and reducing the effects of environmental pollutants. Our emerging capabilities in protein biochemistry and cell signaling are helping to unravel the mechanism by which cells respond to insults, such as radiation, and understanding how inappropriate cellular responses lead to disease, such as cancer. One of our strengths is the integration of experimental and computational techniques into a systems approach to understand complex biological processes at a quantitative level. This will allow us to create realistic simulations of cell behavior to both critically test hypotheses and to rapidly predict their responses to new conditions.

To address critical scientific issues involving complex coupled biological and geochemical processes, an interdisciplinary approach is required that uses state-of-the-art science facilities, a noted strength of DOE Laboratories. For example, the success of our environmental microbiology research is in part due to the multidisciplinary teaming between geochemists, biologists, and physicists. Research in the area of subsurface science is developing a molecular-level understanding of the surface chemistry and reactivity of environmentally important mineral phases and is coupling that research with advanced transport models. Using our expertise and capabilities in biogeochemistry, we will continue to build our understanding

of how metals and radionuclide contaminants can be removed or immobilized in the environment by biological processes. We are focusing on the scientific issues fundamental to understanding the biogeochemical factors and processes controlling the microbial reduction of iron, technetium, uranium, and other contaminants in the environment. Some of the knowledge gained from these studies will provide important insights for making decisions in the cleanup process. For example, our research has discovered that the presence of manganese oxides could greatly reduce the effectiveness of the bioremediation of uranium at DOE waste sites. Pacific Northwest National Laboratory is a major contributor to research under DOE's Natural and Accelerated Bioremediation (NABIR) program.

In addition to the NABIR program, our scientists make major contributions to the Environmental Management Science Program and the Geosciences research program in Basic Energy Sciences. Contributions to these DOE research programs have helped make Pacific Northwest National Laboratory an international leader in subsurface science. A strong computational infrastructure has facilitated the investigation of these complex systems. This computational capability has been combined with an experimental flow cell facility in the Environmental Molecular Sciences Laboratory that allows scientists from around the country to test biogeochemical processes in controlled environments. These flow cells can be manipulated to simulate the complex geology and chemistry of subsurface systems.

The sophisticated tools developed in the Environmental Molecular Sciences Laboratory have provided a strong basis for a new research thrust in systems biology that is strongly aligned with the DOE Genomes to Life program. This systems biology approach is the focus of the Biomolecular Systems initiative. A major goal of this initiative is to understand how cells process information in response to environmental changes. Living cells can detect changes in their surroundings through a complex network of biochemical pathways. To gain a full understanding of these signaling networks requires the development and simultaneous application of many new capabilities, such as technologies that allow rapid identification of proteins. Other advanced technologies being used to understand cellular responses include sophisticated optical instruments that can follow single molecules in living cells and that allow direct measurements of protein-to-protein interactions. In addition, our Computational Biology program is building complex models of cell behavior based on the data obtained from our advanced instrumentation. This capability, together with the implementation of new software tools, has allowed us to investigate extremely complex biological systems.

The Laboratory has developed particularly advanced capabilities in proteomics, which is the study of the complement of proteins expressed by a cell population at a given time or under a specific set of environmental conditions. Our initial work in proteomics has been focused on microbial systems. For example, our advanced instrumentation has been used to 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. The number of proteins expressed at a given



Dynamic Range Enhancement Applied to Mass Spectrometry (DREAMS) makes it possible to obtain much more complete proteome coverage and detect many more low-level proteins of importance to cellular processes.

time is large and covers an extremely wide dynamic range of expression levels, making it difficult to analyze all proteins simultaneously. In response to this difficulty, we have developed a new approach of Dynamic Range Enhancement Applied to Mass Spectrometry (DREAMS) to obtain much more complete proteome coverage and greatly enhance our ability to detect the rare proteins that are usually involved in regulatory processes. This technology is based on a high-throughput methodology and analysis by Fourier transform ion cyclotron resonance mass spectrometry. In addition, by using “accurate mass tags,” peptides as identifiers for each protein, we can characterize the proteome far more efficiently than possible by other techniques.

These capabilities serve as the basis for a proposed Production Proteomics Facility that will provide for the characterization of proteins and protein complexes for scientists within the Laboratory, other national laboratories, and the external research community. The capabilities of this proposed facility will allow for the exploitation of results from gene sequencing projects and will support the DOE network of life science investigators. Our proteomics capabilities, together with our strength in microbiology, support many DOE missions in energy, environment, and national security.

As a part of the Genomes to Life program, we propose to develop new approaches to characterize the functional repertoires of complex microbial communities in their natural environment at the molecular level. The capabilities of our Microbial Cell Dynamics Laboratory will allow manipulation of the growth condition for observation of cellular response and processes under a variety of environmentally relevant conditions. Furthermore, the Laboratory has created a partnership with Oak Ridge National Laboratory and others to establish the Genomes to Life Center for Molecular and Cellular Biology for identification and characterization of protein complexes. This effort will combine beyond-state-of-the-art analytical and computational tools, providing the most sophisticated capabilities for the analysis of protein complexes within the DOE laboratory system.

As is stated in the May 2002 Genomes to Life “DOE Resources and Technology Centers for Biological Discovery in the 21st Century” report, DOE requires new research and enhanced technical resources to meet its systems biology needs. These proteomics and microbial cell dynamics capabilities along with others like computational biology, imaging, and structural biology address these needs. Pacific Northwest National Laboratory is positioned to respond in a timely manner to DOE’s needs for these new research centers.

The delivery of the new 900 megahertz, wide-bore nuclear magnetic resonance spectrometer will stimulate advances in structural biology and allow scientists from around the country to learn fundamental information about cellular mechanisms, materials science, and chemical processes. Scientists at the laboratory are investigating how proteins behave in the walls of cells and how they interact with other cellular components. Information obtained in these studies will provide a better understanding of how proteins carry out complex cellular functions.

The knowledge we gain from the scientific tools developed for systems biology also will enhance our knowledge on the effects of low-dose exposures to ionizing radiation or chemicals. Currently, the health effects of low-dose radiation are not well understood and this issue is of critical importance for setting defensible safety standards for DOE missions, such as nuclear waste treatment and storage strategies. We have developed and characterized a cell irradiator that can mimic effects of

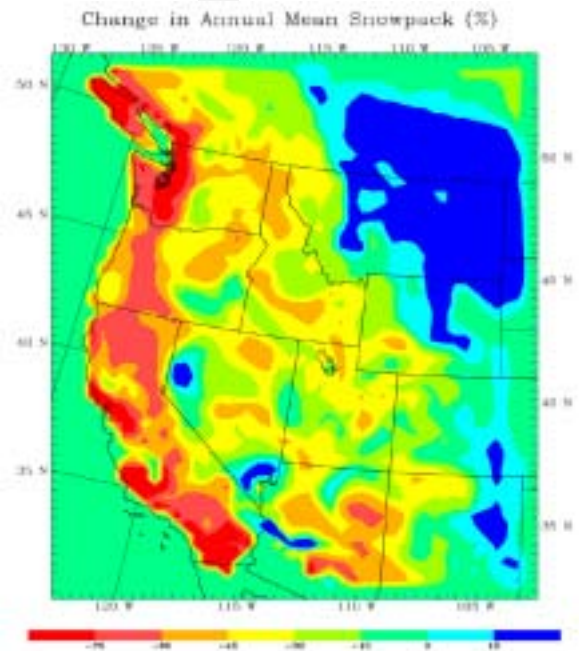
ionizing radiation within selected cells for studying bystander effects and adaptive responses. Combining this instrument with the tools we are building for systems biology will allow observation of cellular and multicellular responses. Researchers also are investigating the molecular events responsible for cellular responses to low-dose radiation and are developing models systems to define thresholds that trigger cell-signaling pathways. New information from these studies can impact our understanding of the linear no-threshold model that is the current basis for low-dose radiation risk assessment.

4.1.2.2 Atmospheric Science and Global Environmental Change

To support the President's National Climate Change Research Initiative and National Energy Plan, our mission in atmospheric science and global change research is to gain a predictive understanding of the fate and effects of energy-related emissions in the atmosphere that will enable the design of effective actions for adaptation and mitigation. Our global change research is making important contributions to improving the modeling of climate processes and to understanding the potential effects of climate change on key natural resources and human activities. In atmospheric sciences, we are playing a key role in the nation's air quality research program by improving understanding of the coupling between meteorology and chemistry and developing new instrumentation for measuring or characterizing important atmospheric constituents. A major portion of our research is focused on the problem of global climate change. Understanding the physics of climate change, as driven by increasing greenhouse gas concentrations, requires a detailed understanding of the multiple feedback processes initiated by the seemingly small changes in the atmospheric energy balance caused by carbon dioxide increases. The most important of these feedbacks involves the impact on the hydrologic cycle, most notably the effects of increasing concentrations of greenhouse gases on the distribution and properties of clouds in this wetter and warmer atmosphere.

The Atmospheric Radiation Measurement program, a DOE multilaboratory effort with involvement of universities and other agencies, is enlarging our understanding of clouds and their impact on atmospheric radiation. The principal goal of the Atmospheric Radiation Measurement program is to improve the representations of these processes in global climate models, and in turn, the quality of and our confidence in simulations of climate change. We will continue to provide leadership for this program in both the scientific and operational components.

In the next few years we expect to play a much larger role in the scientific investigations related to climate change. We will continue research on improving remote sensing of atmosphere and cloud properties, parameterizing cloud processes in climate models, and elucidating the role of surface properties in the formation of clouds. In addition, we have developed a state-of-the-art mobile remote sensing facility, the Pacific Northwest National Laboratory Atmospheric Remote Sensing Laboratory (PARSL), that includes dual-wavelength millimeter radar,



Our regional climate models predict that warming associated with the projected build-up of greenhouse gases may lead to more than 50% reduction in snowpack along coastal mountains, along with increased likelihood of wintertime flooding and decreased summertime water supply in major river basins.

Our groundbreaking work in the development of global-scale integrated assessment models is useful for understanding the policy options available for minimizing and mitigating climate change.

dual-wavelength lidar, and passive radiometry. This facility can be used locally or deployed nationally and internationally to carry out research on atmospheric aerosols and clouds.

We will continue to perform a range of atmospheric research on understanding the regional and global consequences of climate change. Regional and global general circulation models support investigations into how clouds, trace gases, and aerosols affect global climate and how changes in the global climate are expressed at the regional scale. The regional models provide essential coupling between the greenhouse gas drivers and the effect on human systems, such as agriculture and water resources. The regional modeling system developed at the Laboratory will continue to play an important role in assessing climate change effects.

The Joint Global Change Research Institute between Pacific Northwest National Laboratory and the University of Maryland is committed to significantly improve our ability to assess the effects of increasing atmospheric concentrations of greenhouse gases on human activities and the natural environment and to understand the measures that can be most effective in managing the risks associated with these effects. This new effort joins smoothly with research efforts in the Atmospheric Radiation Measurement program and in regional climate prediction, which are both designed to improve our understanding of the physical processes of climate change.

Integrated assessment for climate change assembles knowledge from a diverse set of sources, relevant to one or more aspects of the climate change issue, for the purpose of gaining insights that would not otherwise be available from traditional, disciplinary research. This capability can help us consolidate our understanding of the implications of advances in scientific, engineering, and policy endeavors, and lay the foundations necessary for a rational and effective response to climate change. Through the Global Technology Strategy Project, we will provide an understanding of the potential mitigation options by considering the interrelationships between present and future energy technologies, economic activities, and climate policy.

In atmospheric science, a major obstacle in understanding the fate and effects of energy production is representing effectively the interactions between meteorology and atmospheric chemistry in predictive models. We also have gaps in our understanding of the atmospheric processes that determine the chemical and physical properties of atmospheric aerosols. Aerosols are important factors in such issues as human health, climate change, and the impairment of visibility. Data from recent field campaigns in Arizona, Texas, California, and Utah are being used to investigate the mechanisms responsible for the chemical transformation and vertical movement of pollutants in the atmosphere, especially over urban areas. These studies are of both scientific and practical interest because the results will improve not only our understanding of air quality problems, but also our ability to predict weather in western mountainous areas. In this focus on chemistry, transport, and aerosols, we bring to bear our capabilities in field research, including our Gulfstream 159 aircraft, computational modeling of both meteorology and chemical processes, and the distinctive analytic capabilities of the Environmental Molecular Sciences Laboratory. The latter has focused on developing new instrumentation for measuring or characterizing important atmospheric constituents.

Carbon management is an international issue that impacts our National Energy Policy, and carbon sequestration is a key component of the carbon management strategy. The Laboratory is part of the leadership in the Oak Ridge-Argonne-Pacific Northwest National Laboratory collaboration in the study of the sequestration of carbon in terrestrial ecosystems. Work is under way to identify and characterize links between critical molecular, ecophysiological, and ecosystem processes to better assess and manage sequestration potential and its ecological and socioeconomic impacts.

4.1.2.3 Materials and Chemical Sciences

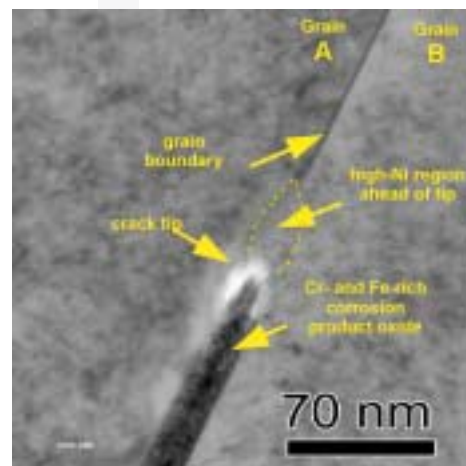
Pacific Northwest National Laboratory will continue to build our internationally renowned expertise in advancing the state-of-the-art experimental, theoretical, and computational tools to describe and model structures and processes of molecular and nanoscale systems in complex environments.

Researchers in chemical structure and dynamics are exploring reaction mechanisms at a wide variety of solid/liquid and liquid/liquid interfaces, high-energy processes at environmental interfaces, cluster models of the condensed phase, the dynamics of biological systems, and development of new analytical methods to detect and characterize atmospheric species. One application of this research is in solving waste management and environmental cleanup problems at contaminated waste sites, in the atmosphere, and in outer space.

Over the past decade, the Laboratory has established itself as a world leader in the synthesis and characterization of novel oxide materials. Molecular beam epitaxy and reactive beam deposition techniques are employed to synthesize thin oxide films ranging from well-ordered single crystals to extremely high-surface-area nanoporous arrays. In related studies, cluster beam and laser spectroscopic techniques are used to synthesize and study the electronic properties of oxide clusters ranging from a few to a few hundred atoms. Collectively, our research is aimed at understanding, and ultimately controlling the chemical and physical properties of these materials at the nanometer scale. Our goal is to utilize this understanding to benefit DOE programs focused on a diverse problem set such as catalysis, energy storage, sensors, and subsurface contaminant migration and mitigation.

In the area of biological processes, sophisticated tools such as single-molecule spectroscopy and high-resolution biological imaging make it possible to detect single molecules at room temperature and to conduct spectroscopic measurements for monitoring their dynamic processes. These tools provide the opportunity to view chemical reactions in a living cell in real time. Single-molecule and single-cell measurements provide real-time data on molecular motions resulting from cell functions and how the timing of these reactions is correlated with other cellular biological activities. Such data will open up many exciting possibilities for probing cellular processes. This will support our new research efforts in systems biology.

Our molecular theory and modeling programs are producing sophisticated and useful methods for studying molecular processes in condensed-phase systems. Aqueous-phase systems are common in DOE waste management problems and, therefore, will continue to be a major theme of these molecular studies. Research includes the study of molecular processes in clusters and liquids, at liquid interfaces,



High-resolution transmission electron microscopy image of crack tip in an irradiated stainless steel. Selective dissolution of iron, chromium, and nickel stainless steel at grain boundaries has been identified as an important and unexpected cracking mechanism under irradiation.

“Many advanced technologies rely on strong interfaces between metals and oxides,” said Scott Chambers, Pacific Northwest National Laboratory scientist. “These findings are very exciting because they may provide the molecular insight industry needs to create better materials for microelectronics and sensors.”

and in covalently bonded materials. New capabilities in the areas of advanced electronic structure methods, reaction rate theories, and accurate interaction potentials for molecular simulations are being developed to make more reliable predictions about complex molecular systems. Development and implementation of new methods and algorithms into the NWChem suite of codes is ongoing. A new program in computational heavy element chemistry is anticipated. These tools will be used to study a variety of problems such as groundwater chemistry, chemistry at aqueous and mineral interfaces, separations chemistry, and nuclear waste forms. The ability to apply advanced theory and experimental approaches to the same complex problem is a key strength of our program.

The Laboratory’s research programs in molecular processes will continue to focus on catalysis and chemical transformation, and separations and analysis. We conduct fundamental studies on the surface-induced dissociation of polyatomic ions, laser-based analytical techniques, chemical and structural principles in solvent extraction (in collaboration with Oak Ridge National Laboratory), solvation and reactivity in supercritical fluids, free radical chemistry at high temperatures and experimental studies of heterogeneous catalysts. Our research on rhodium catalysts has established a more quantitative relationship between surface structure and catalytic activity for the reduction of nitrogen oxide. New programs exploring the reaction specificity of nanoparticles in solution and control of the non-thermal reactivity of metal oxide structures through nanoscaling will be established. Additional programs in nanocatalysis and biocatalysis are anticipated.

Our materials science effort is driven by successful integration of materials modeling activities that guide the development of novel synthesis and processing methods, that direct experimental design in resolving key structure-property relationship issues, and that provide insight to failure phenomena in materials. Leading-edge research on metals, ceramics, polymers, and composites addresses fundamental issues critical to the science mission of the Department of Energy.

Current activities in the now prominent nanoscience and nanotechnology area, which began at this Laboratory well over a decade ago, focus on understanding and tailoring fundamental molecular interactions at interfaces that direct the growth of hierarchically ordered materials. Our long-term goal is to develop self-assembly methods that allow spontaneous formation of ordered structures on different length scales with improved functionality over bulk materials. We support the National Nanoscience Initiative through 1) sustained research programs funded by DOE and 2) internally funded projects designed to promote interlaboratory interactions and create multidisciplinary teams to address critical science issues. The sophisticated scientific tools at the Environmental Molecular Sciences Laboratory will continue to provide world-class support of our research efforts in the nanoscience areas. We plan to develop interactions with instrument development teams at the Spallation Neutron Source and other neutron sources to apply these instruments to study and characterize the nanostructured materials we developed. Through the Laboratory’s Nanoscience and Nanotechnology initiative, we have partnered with the University of Washington to form the Joint Institute for Nanoscience to promote these interactions. The polymers thrust area within the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials, coordinated at this Laboratory, is an important vehicle for nurturing these interactions and establishing links with the more applied DOE agencies and industry.

We excel in the metallurgy and ceramics area, using a combination of experimental and modeling approaches to study chemical and structural defects in these materials and how their presence and distribution affect properties. Research also focuses on the chemistry and physics of interfaces, a good understanding of which would allow intelligent design of materials having tailored properties and chemical reactivity. A long-term goal of these studies is to develop innovative approaches for designing smartness into a material, thereby enabling a reversible change in specific properties in response to changes in the ambient environment.

The integration of small scale architectures and imprinted chemical functionality to an interface will lead to a significant perturbation as to how that interface interacts with the environment. Such smart interfaces may take the form of fibers, patterned surfaces, and three-dimensional constructs such as the interconnected gyroid structure (surface of minimum curvature) observed in phase separated block polymer systems. PNNL staff will leverage previous and ongoing fundamental research results to guide studies aimed at understanding the key structural and chemical factors that are necessary to build a smart interface. The intent of this work is to: identify the controlling factors, structural and chemical, that influence interfacial response; describe innovative processing approaches including self-assembly for the development of these smart interfaces; and apply advanced characterization methods including sophisticated magnetic resonance techniques (hyperpolarized ^{129}Xe NMR) to evaluate interface morphology, local chemistry, and physical response. The basic research pursued here will drive technical thrusts of both the more applications-oriented DOE Program Offices and the commercial sector. The approach is to pursue fundamental science that will serve to underpin future development activities to support the applied program thrusts at the Laboratory.

Electric/magnetic field distributions at architected interfaces are known to influence both specie transport and surface chemical reactions. Understanding how interfaces direct a specific interfacial response is paramount to engineering smartness into the interface. For example, regulation of transport phenomena (electrons, heat, light, chemical species) at an interface is necessary for incremental improvement of: optical and thermo-optical switches for use in smart paints or in color-converting clothing (camouflage); ion-selective membranes for battery and fuel cell applications; intellomeres to promote self-healing and repair of composite structures; phase transformation interfaces to stimulate protein release; and smart insulation driven by modification of resident void size.

A materials-by-design approach is used to drive the synthesis of modified interfaces that have a specific nanostructure and an associated predetermined response to an externally applied force. Modeling studies are undertaken to determine the critical molecular parameters that influence the self-assembly process in synthesizing these systems. Simulation also proceeds on larger-length scales to evaluate the electroactive response as a function of the resident nanoarchitecture. Modeling on various length scales is key for developing structure-property relationships in these phase-separated polymer systems and also provides a rational approach for the synthesis component of the research activity. Property measurements are used to both evaluate the enhanced response and validate the modeling predictions. Critical outcomes of the proposed research include development of a fundamental understanding of the role of phase transitions in forming

Because the boundary between a material and the environment is an interface, prospective research will focus on understanding how both chemical and structural modifications of an interface correlate with interfacial response to an imposed stress.

The challenge to the smart materials task area is to understand how resident chemistry and hierarchical structural organization drive the response of a material to perturbations in the environment.

self-assembled nanostructures, the attendant structure-property relationships, and new approaches to actively regulate transport properties (ions, molecules, heat, light, etc.) in these materials.

Progress in the smart materials thrust area is predicated upon understanding how resident interfacial architectures perturb local electromagnetic field distributions at an interface that in turn direct interfacial response. This activity relies on local field modeling approaches already developed at this Laboratory and refined incrementally over the past dozen years. Modeling results are used to understand how local architectures affect specie transport and local reactivity and how such architectures can be manipulated to magnify field induced effects. For example, the dielectric constant of a void composite material has been shown in simulations and verified experimentally to be highly dependent upon how the voids are organized in the material. Since the optical properties of a material are related to the dielectric response function, they can be altered predictably by tailoring the interfacial architecture.

To understand material response to environmental perturbations, multidisciplinary research in the following areas is mandated: phase transformation dynamics (particularly second order processes) in self-assembled nanostructures; structure-property relationships for these tailored architectures; and innovative approaches to actively regulate transport phenomena. Activities are to be focused on the development of synthesis/processing routes to achieve targeted architectures predicted from simulations to exhibit the desired response to an applied stimulus. Modeling-directed synthesis will invoke traditional organic/inorganic chemistry approaches and will include solid state techniques (topochemical synthesis), “lego” synthesis approaches, and other non-conventional methods. These architectures can be “smart” by themselves, or can attain “smartness” through surface chemical modification (imprinting). This is achieved by invoking phase transformation phenomena, perturbation to resident electronic charge states, stimulated ion transport, solvation, and other processes. Future activities will leverage ongoing research in two multilaboratory research centers that are coordinated at PNNL: The Polymers project (*Smart Materials Based on Electroactive Polymers*), DOE Center of Excellence for the Synthesis and Processing of Advanced Materials; and, the Tailored Nanostructures project associated with the Joint DP/BES NNI Network.

Laboratory activities also pursue mechanical property measurements of materials where studies are carried out under hostile chemical environments, at extremely high temperatures, and in radiation environments to better understand the mechanisms of stress corrosion and corrosion fatigue. This research provides insight to the behavior and reliability of materials that are used in the building industry, power generation industry (ranging from fuel cells to commercial power plants), and in the transportation industry.

4.1.2.4 Computational Science

We are building our computational science program around focused research efforts in specific application areas, or the concept of Topical Computing Facilities, as outlined by DOE’s Scientific Discovery through Advanced Computing (SciDAC) program. The Molecular Science Computing Facility in the Environmental Molecular Sciences Laboratory is the prototype Topical Computing Facility with its focus in chemistry, biochemistry and biophysics, environmental science, and nanoscience. Following the model of the Molecular Science Computing Facility,

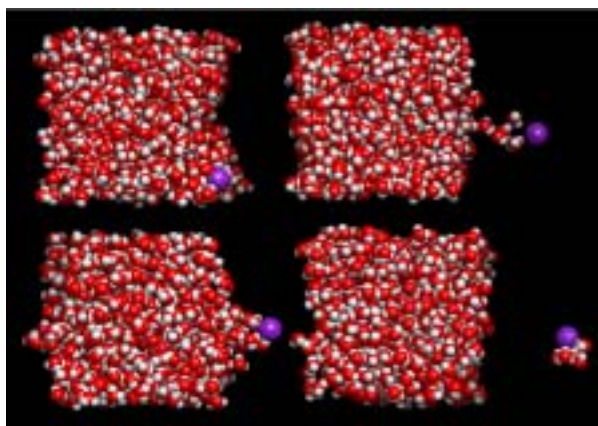
our goal is to lead or be a major partner in Topical Computing Facilities in computational biology, subsurface reactive transport, and regional climate modeling. These Topical Computing Facilities are founded on core basic science expertise, which is described below.

The Molecular Science Computing Facility supports our core science areas of molecular structures, reaction energetics and kinetics, and spectroscopy with applications to environmental science, interfacial science, catalysis, and nanoscience. We have strong efforts in computational and theoretical chemistry focused on interfacial phenomena; aqueous chemistry; new methods development for high accuracy on complex molecules; computational geochemistry and biogeochemistry; relativistic quantum chemistry; computational thermochemistry, kinetics, and spectroscopy; and computational nanoscience from the molecular level toward the bulk. For example, in collaboration with Argonne National Laboratory and the University of California–Davis, we have determined a new heat of formation for the hydroxyl radical, a key species in combustion processes and in atmospheric reactions. We will continue to study the interactions of complex biomolecules on the surface of bacterial membranes with mineral surfaces relevant to environmental cleanup processes. By combining high-level quantum chemical calculations with detailed experimental measurements, we predict the structures and speciation of different species to develop accurate models of the thermodynamics of compounds in the Hanford waste tanks.

To meet the ever-increasing science needs of the Molecular Science Computing Facility to address the computational grand challenge problems in environmental science, we are significantly upgrading (with funds from the Office of Biological and Environmental Research) the current high-performance computer system. Replacing this 5-year-old system is a \$24.5 million Hewlett-Packard Linux-based supercomputer. Installed in August and September 2002 at the Molecular Science Computing Facility within the Environmental Molecular Sciences Laboratory, the supercomputer will allow Environmental Molecular Sciences Laboratory researchers and users to study more complex chemical problems that form the basis for new discoveries in biological systems, subsurface transport, atmospheric chemistry, catalysis, combustion, and material design. The massively parallel computer consists of 1,400 next-generation Intel processors with an expected total peak performance of more than 9.1 teraflops.

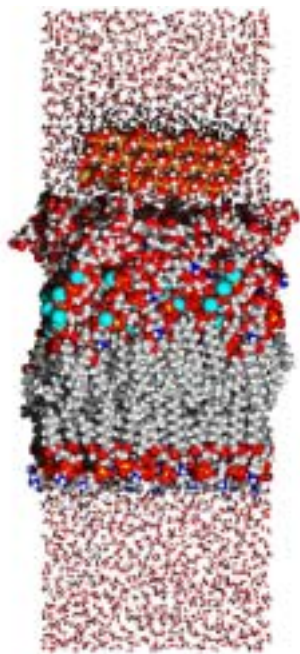
We are building a strong program in computational biology with a focus on modeling protein-protein interactions, new tools and methods for genomics and proteomics analysis, modeling of intra- and extra-cellular pathways including signaling and advanced spatial analysis of cells based on new imaging methods, discrete mathematics for biology, and the development of a collaborative problem-solving environment for biologists. Much of the effort is focused on microbial systems relevant to environmental remediation and energy security.

Our expertise in subsurface reactive transport is applicable to a wide range of pollutant transport problems including the vadose zone at the Hanford Site. Highly resolved depictions of the effects of physical and chemical heterogeneities on subsurface flow, transport, and reactions have been used to simulate the behavior



Molecular dynamics simulations allow accurate characterization of the molecular mechanism of anion binding to the interface of water. Here an iodine anion moves from the vapor/liquid interface of water to the vapor phase.

The Pacific Northwest National Laboratory's new Linux-based supercomputer is the world's largest Linux cluster, providing a unique computing environment for our users to conduct their science, and increased capacity to better serve the user community.



We are modeling the interactions of lipopolysaccharides (LPS) located on the outer membrane of gram-negative bacteria with mineral surfaces and how such interactions affect metal uptake and mineral dissolution. This shows a molecular representation of the LPS membrane of *Pseudomonas aeruginosa* in near contact with the goethite mineral fragment.

Topical areas in computational science, with the accompanying foundation in applied mathematics, statistics, and computer science infrastructure, will continue to play a fundamental role in all of our research endeavors.

of leaks from the high-level waste tank SX-109 at Hanford, including mineral dissolution and precipitation as well as to model biogeochemical reactive transport. Fundamental information to predict the fate and transport of contaminants arise from our strong basic science program in environmental microbiology and geochemistry as evidenced by our contributions to DOE's Natural and Accelerated Bioremediation (NABIR) program, the Environmental Management Science Program (EMSP), and the Basic Energy Sciences Geosciences program. A Topical Computing Facility in Subsurface Science will ensure that fundamental science developed by these basic research programs will be used to predict the fate and transport of contaminants and enable technical and policy decisions with respect to waste management and cleanup at DOE sites.

We are making several contributions in atmospheric reactive transport and regional climate modeling. Global climate change affects critical environmental resources and human activities at the regional scale. To understand these problems requires information at temporal and spatial scales that are beyond the capabilities of current global climate models. Models are needed to evaluate the next generation of subgrid-scale process packages for high-resolution climate models currently under development. This includes atmospheric chemistry models, such as the PEGASUS model. This Eulerian air chemistry model was developed for massively parallel computers to evaluate the influence of stratospheric intrusions of air upon surface ozone concentrations in urban environments. The much higher resolution of this code allows improved chemistry models to be included and comparisons made to observational data.

In applied mathematics, we have three core thrusts in the Laboratory. The first is built around a core expertise in discrete mathematics, combinatorics, and graph theory, as applied to discrete, deterministic complex systems networks modeling and simulation. This effort will play a key role in systems biology in terms of network analysis in cells and in communities of cells and in the analysis of economics-driven electric power grids and maintaining the energy security of the nation. The second is focused at the juncture of computational mathematics, numerical methods, and numerical analysis. Key application areas include using multiresolution analysis methods in computational chemistry to enable fast electronic structure methods with controlled precision and in solving advection-diffusion equations and time-dependent simulations (e.g., Navier-Stokes for fluid simulations). The third area is the development of new grid generation techniques with the accompanying solvers for computational physics in complex geometries for massively parallel computer architectures. This effort is built around the codes NWGrid (grid generation) and NWPhys (physical equation solvers), which are incorporated into the P3D system. Our statistics effort will focus on the design, assessment, and uncertainty management for these modeling and simulation efforts.

We envision playing a leadership role in two key areas of computer science. The first is the fundamental computer science needed for collaborative problem-solving environments with two components: 1) distributed data architectures, data management, data mining, and scientific data modeling; and 2) component architectures for software design. The second area is enabling high-throughput, high-performance computing on massively parallel processing computer architectures. This area also has two components: 1) development of tools and methodologies for applications to run on advanced parallel architectures, and 2) system software and tools to deliver maximum performance to the user on

massively parallel processing architectures. The first software development effort builds on the ParSoft set of paradigms for managing the complex memory hierarchy in massively parallel computers. With our Global Arrays shared-memory programming environment, scientists from a range of computational disciplines—computational chemistry, computational biology, fluid dynamics, and data mining—will be able to adapt their software to parallel computers efficiently. This reduces time and programming effort for software conversion and enables scientists to tackle larger and more sophisticated computational problems in the parallel computing environment. In the second area, we are developing capabilities to enable high-throughput computing on massively parallel processing architectures for large-scale simulations in a batch computing mode where we envision using significant fractions of a large massively parallel processing computer for simulations.

4.1.2.5 User Facilities

Pacific Northwest National Laboratory provides world-class facility and instrumentation for the scientific user community. Notables are the Environmental Molecular Sciences Laboratory, the Atmospheric Radiation Measurement program, and the Gulfstream 159 aircraft.

The Environmental Molecular Sciences Laboratory offers—at one location—a comprehensive array of leading-edge resources for research in the environmental and molecular sciences. Users may define combinations of equipment and capabilities from six facilities that best meet their own special needs. Resident scientists and engineers provide a network for collaboration with users. Over 1,400 scientists from universities, other national laboratories, and industry used the Environmental Molecular Sciences Laboratory during its fourth year of operation (see Table 4.2). At the Environmental Molecular Sciences Laboratory, our scientists develop molecular-level understanding of the physical, chemical, and biological processes that underlie critical environmental issues.

Resources available to users and resident staff include the

- Advanced Monitoring and Detection Facility for monitoring and detecting trace species in complex matrices
- High-Field Magnetic Resonance Facility for structural biology and micro imaging

The Environmental Molecular Sciences Laboratory capabilities support all major DOE science missions, environmental management, national security, and energy. The Laboratory is working with the DOE Office of Science to develop a description of areas of special emphasis.

Table 4.2. Environmental Molecular Sciences Laboratory Users - 2001

	Number of Users	Number of Organizations	Percentage of Use
Laboratory	229		16
Other Federal Laboratories	135	17	9
University (U.S.)	886	132	63
Industry (U.S.)	165	55	12
Total	1,415	204	
Remote Users	784		55
Visiting Users	631		45
Total	1,415		

- High-Field Mass Spectrometry Facility for analyzing biomolecules and their response to environmental stimuli
- Interfacial and Nanoscience Facility for fabricating and characterizing materials and systems with dimensions on the nanometer length scale and studying interfacial chemical reactions and processes
- Molecular Science Computing Facility for computational simulation of complex phenomena
- Optical Imaging and Spectroscopy Facility for developing and using advanced optical techniques to characterize complex systems.

Also, the Environmental Molecular Sciences Laboratory facilitates remote collaboration, and the Instrument Development Laboratory works with scientists to develop custom electronics and software to meet specific research needs.

Additional resources will be available in the future within the scope of the proposed systems biology research centers. These proposed resources will be in direct support of the May 2002 Genomes to Life “DOE Resources and Technology Centers for Biological Discovery in the 21st Century” report. The initial focus of these research centers will be a high-throughput Proteomics Laboratory and a Microbial Cells Dynamics Laboratory. Other potential systems biology research centers include an imaging resource and a strong program in computational biology.

The Laboratory is a key participant in managing and operating the climate research monitoring stations of DOE’s Atmospheric Radiation Measurement program in Oklahoma, the North Slope of Alaska, the Tropical Western Pacific and Australia. The Atmospheric Radiation Measurement program uses remote-sensing instruments to study cloud physics. These instruments include millimeter-wavelength radar and Raman lidar that are operated continuously and with high accuracy to sample atmospheric properties. Atmospheric data also are obtained using aircraft and satellites equipped with instruments. The data management facility in Richland oversees the data collection process and develops new computation algorithms to retrieve more complex information from the various data streams. The program office coordinates the multilaboratory and external

research and ensures that the Atmospheric Radiation Measurement facilities are available to and used by a broad spectrum of scientists in the climate change, atmospheric research, and satellite remote-sensing communities.

Pacific Northwest National Laboratory operates a Gulfstream 159 research aircraft for studying atmospheric processing and contaminants. Operated since 1995 as a DOE research aircraft facility, the Gulfstream 159 has been host to investigators from several DOE laboratories and universities in studies of the chemistry and physics of air pollution in major urban areas of the United States. As an airborne atmospheric chemistry research laboratory, the Gulfstream 159 has been used to test new analytical instrumentation for gaseous and particulate pollutants and to measure the horizontal and vertical



The new Atmospheric Radiation Measurement site at Darwin, Australia, will expand our understanding of regional climates.

distributions of primary and secondary pollutants aloft. Observations from the Gulfstream 159 have provided important information on the production of ozone in urban and power plant plumes that will help the design of effective emissions control strategies for this pollutant. The current focus is on bringing new instruments on board for investigating the chemical composition of gaseous organic and fine particulate matter.

4.1.2.6 University and Science Education Programs

The University and Science Education programs at Pacific Northwest National Laboratory strengthen working relationships with universities and enhance our basic science capabilities. With strong support from the DOE Office of Science, we partner with universities on major research programs; provide opportunities for visiting university faculty, students, graduate students, and postdoctoral fellows to work at the Laboratory and gain research experience; and participate in educational and research activities, such as joint institutes, at other campuses. Further details are provided in the Operations and Infrastructure section.

4.2 Environmental Quality

Pacific Northwest National Laboratory's diverse science and research capabilities and depth in environmental science and radiological materials and operations serve an essential role in supporting the critical national mission of cleaning up the legacy of nuclear weapons production. The science and technology requirements to appropriately address environmental cleanup are daunting. The Department of Energy faces major challenges and responsibilities for sites that contain enormous amounts of solid radioactive and hazardous waste buried in the subsurface, millions of cubic meters of contaminated soil, billions of gallons of contaminated groundwater, massive contaminated structures, and millions of gallons of high-activity radioactive waste stored in large underground tanks. These challenges require forefront technologies to efficiently and cost-effectively carry out the cleanup process, and the Pacific Northwest National Laboratory is committed to fully supporting DOE's Accelerated Cleanup and Closure Strategy.

4.2.1 Strategic Intent

The Pacific Northwest National Laboratory will continue to be a leader in providing the science and technology necessary to address the Department of Energy's critical environmental quality issues. We will do this through the strength of our capabilities and through strong and strategic partnerships with others to ensure the best resources are brought to bear on our national environmental cleanup problems.

We will play a major role in providing the science and technology needed to manage, process, and dispose of radiochemical legacy materials throughout the DOE complex, and we will continue to provide high-quality leadership for DOE's high-level waste program.

We will continue to accelerate the accomplishment of DOE's environmental cleanup goals. Our advanced computational capabilities will enable us to design biochemical remediation processes that target specific distributed contaminants, optimize the facilities that will be used to treat large quantities of concentrated

Our science and technology contributions will substantially reduce the cost, time, and risk associated with DOE's cleanup, and will enable site cleanup and closure decisions to have a sound, scientific basis.

contaminants, and provide credible, defensible, rapid, and visual subsurface contaminant behavior models that satisfy all stakeholder needs for decision and informational tools.

The tools and technologies we develop for cleanup will also be expanded to help address this region's, and the nation's, most challenging natural resource issues—water stewardship, carbon management, and ecosystem protection. Through advanced computation, we will design optimal water use approaches and, teaming with basic science experiments, we will develop new treatment technologies that fundamentally improve the way we ensure clean water. In the carbon management and ecosystem protection areas, we will develop novel capture, sequestration, and passive monitoring systems that will be scalable such that they have a dramatic effect on protecting our planet. Through partnerships with leading agriculture universities and industry leaders, we will fundamentally change 21st century farming and crop processing practices. Using an integrated computational, experimental, and production scaling program, we will advance this nation's ability to produce



We will develop financially attractive systems that use biomass to produce industrial and consumer products.

biomass economically and in an environmentally sustainable manner, and to transform it into high-value chemicals and products.

Pacific Northwest National Laboratory will support the Core Laboratories planning efforts to bring the best science and technology to bear on critical environmental quality challenges at multiple sites, and where a complementary research agenda will prove beneficial for cleanup. As part of this effort, we intend to provide our capabilities to all environmental quality areas where we are suited, including a leading role in subsurface computational science.

At the national level, the Laboratory will continue our leading role in linking environmental science to technology through effective deployment of Environmental Management Science Program results and by building strong linkages to Office of Science environmental science programs.

To demonstrate our environmental management and stewardship commitment to current and future clients, we will seek independent third-party registration of our environmental management system to the ISO 14001 Standard, in 2002. The ISO standards, including the environmental management system Standard ISO 14001, promote free trade and the sharing of ideas and technologies in the world market. The ISO 14001 Standard specifically recognizes that a healthy environment is necessary for continued economic and scientific development.

At the Hanford Site, we will continue to lead the delivery of the scientific and technical basis for Hanford cleanup decisions and long-term stewardship while partnering to provide innovative solutions to crucial problems—such as special nuclear materials disposal and groundwater cleanup. The Laboratory will support Hanford's Accelerated Cleanup and Closure Strategy and promote revolutionary

breakthroughs in treating Hanford tank wastes. Through appropriate partnerships with Site contractors and others, we intend to play a major role in providing the science and technology necessary to ensure that baseline Hanford tank cleanup challenges are addressed. The key to delivering resourceful technology solutions to the most difficult environmental challenges will be strong, science-based programs, such as the Environmental Management Science Program and the advanced research conducted at our strategic facilities:

- Radiochemical Processing Laboratory—one of just two facilities in the nation available to support DOE multiprogram national research in radiochemical processing; it houses specialized facilities supporting radiochemical process development, chemical and physical separations, thermal processing, radio-materials characterization, radioisotope production, and analytical chemistry.
- Environmental Molecular Sciences Laboratory—provides tools and advanced resources for developing a molecular-level understanding of fundamental physical, chemical, and biological processes, including atmospheric chemistry, cellular response to environmental contaminants, contaminant fate and transport, and waste processing.

The success of our research will depend on the continuing availability and advancement of specialized instruments in these laboratories along with trained and experienced staff.

The Fitzner/Eberhardt Arid Lands Ecology Reserve has been used as an ecological research area since 1965. The Arid Lands Ecology Reserve became a Federal Research Natural Area (Rattlesnake Hills Research Natural Area) in 1971 and was designated a National Environmental Research Park in 1977. The Arid Lands Ecology Reserve is one of seven National Environmental Research Parks established at DOE sites to advance the nation's goals of restoring, protecting, and enhancing environmental quality. It continues to be a critical field research laboratory for biological, physical, and chemical sciences supporting the Laboratory's programmatic and educational efforts.

At the present time, about 10 active science and education projects (some supported by Arid Lands Ecology Reserve facilities) are under way supporting both Environmental Management and the Office of Science. Examples include ecology, meteorology, global climate, geology, seismology, hydrology, cultural resources, physics, astronomy, and a range of education outreach activities. The Arid Lands Ecology Reserve's value as an environmental laboratory is priceless, serving not only as an experimental and educational facility, but also as a minimally affected regional reference environment against which the impacts of energy development and use plus cleanup of the nearby Hanford Site can be measured and predicted.

Historically, our partnerships included a number of universities and non-DOE agencies such as the U.S. Environmental Protection Agency, U.S. Geological Survey, University of Washington, Washington State University, Washington State Department of Fish/Wildlife, and The Nature Conservancy.



As the nation's needs for clean, efficient energy production and use increases, and DOE's environmental cleanup program accelerates, the importance of the Arid Lands Ecology Reserve as a research facility supporting the Laboratory's programs to monitor and predict environmental changes, train the next generation of scientists, and educate the public will increase.

4.2.1.1 Clean Up the Legacy

Pacific Northwest National Laboratory will continue to deliver innovative and efficient solutions and vital environmental knowledge to advance DOE's most pressing cleanup needs in the environmental quality research and development portfolio. Priorities include effectively cleaning up legacy waste materials, disposition of wastes and unneeded materials, and managing future risk.

4.2.1.2 Environmental Remediation

Paramount to successful environmental remediation is the ability to perform cleanup effectively and in the most cost-efficient manner possible, where risks to worker health and safety and the environment are minimized. Pacific Northwest National Laboratory is working to support these objectives through several efforts.

4.2.1.3 Groundwater/Vadose Zone Integration Project

Pacific Northwest National Laboratory is involved in all activities of the Groundwater/Vadose Zone Integration Project, which evaluates future impacts of contaminant movement through Hanford's subsurface and ultimately into the Columbia River. DOE established the Integration Project in 1997 to provide a science-based approach for protecting the Columbia River, which is fundamental to the Hanford Site cleanup effort. The key elements of the Integration Project include site-wide integration of information, the capability to assess the cumulative long-term impact of Hanford-derived contaminants, the development and application of science and technology to address critical Hanford cleanup needs, meaningful public involvement, and extensive expert technical reviews for all Hanford vadose zone and groundwater work. Our Laboratory leads two of the six primary Integration Project endeavors, including science and technology and development and application of the systems assessment capability. Our leadership within the multilaboratory science and technology role is essential, because many uncertainties and data gaps limit our knowledge of the inventory, distribution, and movement of contaminants in the vadose zone and groundwater beneath the Hanford Site. We need to better understand how contaminants move through soils and groundwater, and we are working to identify effective and appropriate methods to dramatically limit this migration. The plans for accelerating cleanup at Hanford include developing new technologies and scientific understanding to treat contaminated soils and groundwater. Current pump-and-treat remediation systems are not sufficient to meet long-term cleanup objectives.

The Systems Assessment Capability is designed to provide technical assessments at multiple levels, including an overall assessment of the impacts and risks associated with Hanford Site contaminants, and will enable the determination of the cumulative long-term impacts of Hanford-derived contaminants on the Columbia River and the Northwest. The Systems Assessment Capability involves an expanded evaluation and methodology to communicate risk from Hanford's contaminants, which includes human, ecological, sociocultural, and economic health factors, in a manner that supports Site cleanup priorities and potential end states.

Pacific Northwest National Laboratory's In Situ Redox Manipulation (ISRM) technology (a passive, award-winning cleanup system for stabilizing or detoxifying contaminants before they reach the Columbia River) is proving safe to implement and will require minimal long-term maintenance. The technology is being applied

at the Hanford Site to treat underground plumes of hexavalent chromium and prevent their migration to the Columbia River. In Situ Redox Manipulation is becoming a recognized model for advanced cleanup technologies due to its effectiveness and increased safety benefits for Site workers.

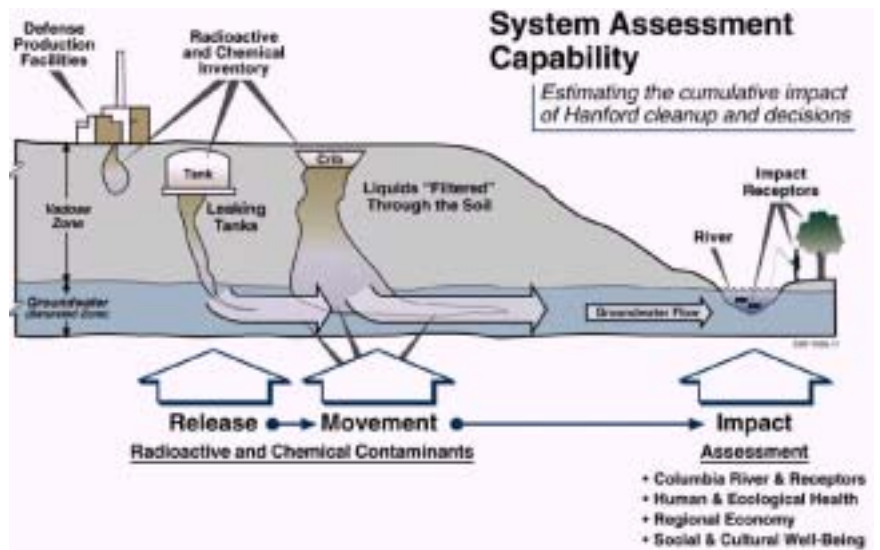
Pacific Northwest National Laboratory manages the Hanford Groundwater Monitoring Project for DOE, and provides integrated, site-specific and site-wide assessments of groundwater quality on the Hanford Site through an integrated groundwater sampling, analysis, and computer-modeling program. This project is part of the Hanford effort to verify compliance with applicable environmental and other statutory obligations.

The project also characterizes and defines trends in the subsurface environment, establishes baselines of environmental quality, and identifies and quantifies new or existing environmental quality problems.

Several Environmental Management Science Program projects support the Integration Project. Most of these projects focus on characterizing the vadose zone in the Hanford tank farm area to determine future corrective measures, including tank waste retrieval strategies. Environmental Management Science Program investigators have received samples of Hanford sediments and are collecting and analyzing data in field experiments. The expertise provided by these scientists from across the United States enhances collection of data that are vital to the Integration Project and increase our knowledge of the vadose zone. Some of the Environmental Management Science Program achievements include

- immobilizing radionuclides in the vadose zone through incorporation into solid phases
- developing radar methods to determine moisture content in the vadose zone to improve characterization methods
- developing improved methods to characterize the subsurface using magnetotelluric inversion codes.

Research supported through fundamental science programs is helping to develop a molecular-level understanding of the surface chemical and reactivity of environmentally important mineral phases. This knowledge can be incorporated into advanced transport models. This research may result in new strategies to control or mitigate the effects of subsurface contaminants. As an example, microorganisms have long been recognized as critical to the conversion of organic materials in the subsurface, and are increasingly being recognized as dominant catalysts in the dissolution and precipitation of minerals. As another example, iron minerals play a major role in the reduction of metals and radionuclides at contaminated DOE sites. Research aimed at understanding the mechanisms and rates of bioreduction of iron minerals is key to predicting and potentially controlling these processes in the field.



The System Assessment Capability model estimates the cumulative impact of Hanford residual contaminants from their source to an accessible environment in the region.

Pacific Northwest National Laboratory researchers are directly involved in 43% of all Environmental Management Sciences Program awards directed at DOE's high-level waste legacy, and approximately 23% of all awards related to subsurface contamination.

4.2.1.4 Subsurface Science

The application of targeted science and technology toward effective environmental cleanup proves instrumental as federal agencies and key audiences balance the need for steady progress given pressing budget constraints. New knowledge, that contaminants formerly believed to be immobile may migrate in the subsurface based on a complex set of environmental conditions, demonstrated the need for new research to support environmental cleanup. Increased knowledge from subsurface and environmental science research will provide the scientific basis for credible and defensible cleanup decisions and will enable effective environmental remediation at DOE's highest priority sites. The same information also will provide the foundation for end-state selection and future stewardship requirements as well as minimize the impact of cleanup activities. The Laboratory will continue to be a leader in new science and research in this area. A focus of our research will be to develop improved science-based cleanup practices and to develop new technologies that are more effective and safer for site workers.

The Pacific Northwest National Laboratory in partnership with the Office of Environmental Management's Core Laboratories, led by the Idaho National Engineering and Environmental Laboratory, actively supports development of an integrated subsurface science and technology effort. The Environmental Management's Core Laboratories with Pacific Northwest National Laboratory's strong support will provide the essential knowledge base and capabilities in five key areas important to achieving the success of identified accelerated and baseline improvement cleanup projects:

- understanding basic subsurface processes
- enhancing data collection and monitoring capabilities
- providing the technical basis for risk-based cleanup decisions
- developing innovative remedial options that are quicker and cheaper while maintaining cleanup quality
- establishing needed accessible computational capabilities with new simulation and numerical models, predictive capabilities, and data visualization methods necessary to communicate results to regulators and stakeholders.

In supporting Environmental Management's project-driven Thrust I and Thrust II research and development agenda, we will investigate the fundamental properties and processes of the subsurface, including the ability to quantitatively characterize and monitor the coupled chemical, geological, and biological processes that drive contaminant migration, and to address temporal and spatial scaling issues that directly affect our ability to defensibly predict and simulate contaminant fate and transport over time and distance. Scaling will be an important component because it represents an impediment to addressing subsurface contaminant behavior and a major research opportunity. The knowledge gained in increased understanding of subsurface phenomena also will be applicable to the future management of natural resources, including oil, gas, and water and the potential reactive transport of terrorism materials.

4.2.1.5 Safety and Health Risks

Inherent to the environmental remediation of the nuclear materials production legacy has been the human health and environmental risk challenges associated with nuclear materials. DOE has a strong history of supporting radiological protection science and technology. Today, the health and safety focus also includes beryllium, lead, arsenic, and other hazardous substances. New technology will need to address worker safety issues, particularly in the area of chemical exposures. Pacific Northwest National Laboratory is a recognized leader in chemical exposure assessment technology development and research. We will apply science from existing disciplines and programs and emerging initiatives to develop technology to advance the protection of workers engaged in the most complex and threatening cleanup missions. By leveraging capabilities in biological sciences, nanotechnology, and sensors, we will enhance worker protection technology. The Laboratory will develop prototypes of the next generation chemical exposure monitors for application initially at Hanford and then for application throughout the DOE complex. We will focus on exposure characterization instrumentation and sensors and biomarker research. Biomarkers will include genomic and proteomic technologies to identify chemical or radiation exposures, response, and susceptibility. Integrating the experimental data into mathematical models will facilitate predicting biological outcome at the molecular, cellular, tissue, organ, and whole organism levels.

The Laboratory is engaged in a number of research activities that align with efforts in worker monitoring and protection, including development of a new, noninvasive technique, building on our ongoing breathalyzer development work, which quickly determines exposures to contaminants using saliva samples. This project, undergoing bench-scale laboratory testing, offers several promising benefits. The technology is designed to be portable, highly reliable, quick in providing results, and cost-effective for on-site monitoring of trace metals and organics. Initial efforts are focused on lead monitoring, but Laboratory scientists are extending the approach to evaluate occupational and environmental exposure to complex mixtures of toxic metals and chlorinated organic compounds. The use of saliva is particularly beneficial, as samples are readily attainable and can be used to quickly screen more individuals than can conventional biomonitoring approaches.



Dr. Steve Miller, Battelle's Inventor of the Year for 2002, was the first person to experimentally observe and develop optically stimulated luminescence.

4.2.1.6 Manage High-level Waste

Pacific Northwest National Laboratory is engaged in high-level waste management activities across the DOE complex to assist in site cleanup and closure. High-level tank waste, a byproduct of the nation's nuclear weapons development program, represents DOE's largest and most complex environmental cleanup challenge, with 60 percent by volume of the total radioactive waste found in the United States located at DOE sites. Pacific Northwest National Laboratory is engaged in high-level waste management activities across the DOE complex to assist in site cleanup and closure. The Laboratory's primary contribution to the high-level waste issues is its support to DOE's Office of River Protection at the Hanford Site near

Richland, Washington. The Laboratory is also engaged in delivering technical support to high-level waste programs at other DOE sites. Our technical contributions to resolving high-level waste issues include:

- collaboration with Savannah River Technology Center to develop a new waste glass formulation with higher waste loadings for implementation within the Defense Waste Processing Facility
- collaboration with Idaho National Engineering and Environmental Laboratory to determine the behavior and mitigation measures of mercury volatilization during vitrification operations
- providing the technical basis for design and operation of retrieval equipment to maximize sludge removal from Savannah River high-level waste tanks
- deploying the prototype system for on-line strontium/transuranic monitoring in support of the monosodium titanate removal process at the Savannah River Site.

Pacific Northwest National Laboratory also continues to provide direct technical support to the West Valley Demonstration Project in West Valley, New York. Serving an important role since 1982, the Laboratory has been providing key technical support for process design and operations, including melter design, canister decontamination chemistry, and cesium ion exchange technology. With vitrification operations now completed at West Valley, we are currently transforming our technical support capability into the decontamination and decommissioning phase.

4.2.1.7 Office of River Protection

Pacific Northwest National Laboratory assists the Office of River Protection by providing technical support to DOE for the planning and management of the Hanford Tanks cleanup mission, and to the two prime contractors for the execution of that mission. The CH2M HILL Hanford Group is the prime contractor responsible for tank farm operations and waste storage and handling, and Bechtel National Inc. has responsibility for design, construction, and commissioning of a \$4 billion Waste Treatment Plant. We also indirectly support the Office of River Protection through our modeling of tank waste releases, their transport through the environment and the estimation of risk from exposure to these releases under the Hanford Site wide groundwater/vadose zone integration project. In our work for DOE directly, we assemble and lead independent technical reviews of the contract deliverables from the Waste Treatment Plant contractor. These reviews include the research and technology-testing program plans and results, the process flowsheet modeling results, and the design optimization studies. We assist DOE in finding new ways to achieve major cost and schedule savings through better technology planning, life cycle analysis, and risk assessment work on various cleanup and closure scenarios.

In close collaboration with DOE and the CH2M HILL Hanford Group project for mission analysis and technology integration, we help to identify, propose, and plan a set of project initiatives that accelerate the cleanup and support the overall plan for the Hanford Site Central Plateau cleanup strategy. We also help to ensure technical integration of Hanford's high-level waste cleanup plans with the overall site cleanup plans and activities along the River Corridor through our unique role in supporting the planning, integration, and assessment work for the DOE Richland Operations office and the Office of River Protection.

Several major research facilities provide unique capability and testing support for the River Protection Project. They include

- Radiochemical Processing Laboratory (RPL)—a hazard Category II nuclear facility for characterizing radioactive waste and waste form samples and validating treatment processes flowsheet options through actual bench-scale radioactive tests
- Applied Process Engineering Laboratory (APEL)—chemical process development laboratory with wet chemical laboratory and large high bay capability for bench through pilot-scale development and process testing with nonradioactive waste simulants
- Environmental Molecular Sciences Laboratory (EMSL)—analytical research laboratory for fundamental studies including computational modeling of waste treatment process chemistry, waste storage behavior, waste form performance, and subsurface transport of waste species
- Fluid Dynamics Laboratories (336 and 338 buildings)—providing simulant development, pulse jet mixer model validation, flow loop studies for waste transfer behavior, and deployment support to waste retrieval activities.

Other areas where we support the Office of River Protection prime contractors include

- assisting the Tank Farm Operations contractor, CH2M HILL Hanford Group, in demonstrating technologies for effective and affordable safe storage, processing, and retrieval of problematical wastes from the oldest single-shell storage tanks and newer double-shell tanks, including inspection, leak detection, and mitigation technologies
- supporting the Waste Treatment Plant contractor, Bechtel National Inc., with the process flowsheet verification using simulated and actual radioactive waste samples, thereby providing essential data and critical insights into how the various process systems will perform
- in partnership with the Tank Farm Operations contractor and the Environmental Management Office of Science and Technology, delivering important scientific knowledge of fundamental waste characteristics, such as providing a better understanding of the relationship between waste chemistry and corrosion of the steel tanks; and developing new technology approaches to lower worker exposure during complex waste handling and tank farm operations tasks, such as the Pit Viper system for robotic operations and maintenance of the waste transfer valve pits.

4.2.1.8 Management of Nuclear Materials

The key technical challenges of nuclear material management include the need for safe and cost-effective processes for characterization, stabilization, packaging, and monitoring/surveillance to minimize worker exposure and meet safeguards, transportation, and verification requirements. At Hanford, Pacific Northwest National Laboratory is supporting site closure activities including the application of science and technology to mitigate the technical challenges associated with stabilization, enhanced storage and the ultimate removal of plutonium-bearing materials, spent nuclear fuel, cesium/strontium capsules, and other forms of special

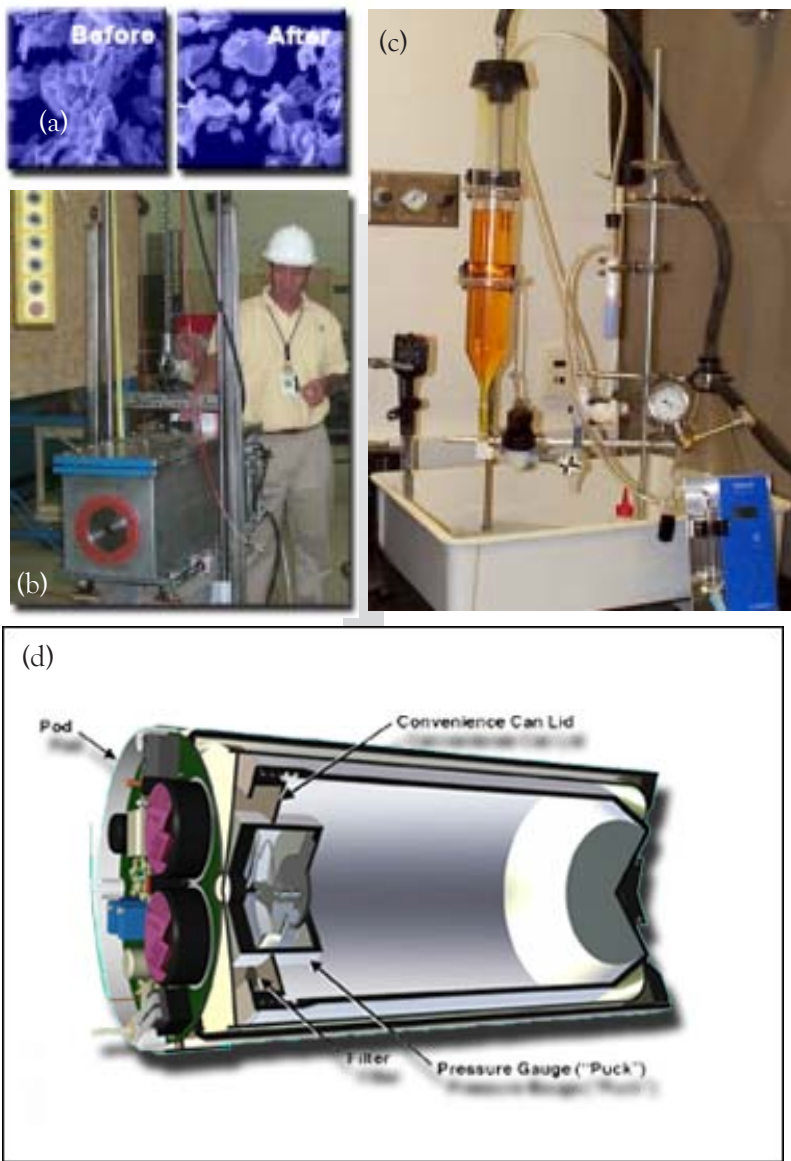
nuclear materials including nearly 4 metric tons of plutonium, 2,100 metric tons of spent nuclear fuel, 47 million curies in the cesium capsules, and 20 million curies in the strontium capsules. Our capabilities in remote handling technologies, radiochemistry expertise, and understanding of radioactive waste inventories and behaviors are valuable resources for the on-site contractors and DOE.

Through formal agreements with on-site contractors such as Fluor Hanford, we are providing direct technical support to the projects, coordinating outreach to the external science and technology community, verifying technical baselines, and providing scientific data to support end state, endpoint decisions for site closure. We are working with Fluor Hanford on enhancing methods for stabilizing more than 4,000 liters of plutonium-bearing solutions in Hanford's Plutonium Finishing

Plant-leftovers from Hanford's production era—using magnesium hydroxide and other precipitation processes. The material is being prepared for long-term disposition at DOE's Savannah River Site. With the precipitation process, plutonium is removed from the solution, processed to a powder, and stabilized in a muffle furnace before placement in three stainless steel containers, one nested inside another. Since many different solution types make up the inventory, the Laboratory is providing testing and laboratory support necessary to optimize separation processes. Pacific Northwest National Laboratory is also providing laboratory testing and process modeling to optimize the stabilization process for more than 1,600 polycubes (2-inch cubes of plutonium that were fabricated in polystyrene in the 1960s) and providing alternative methods to monitor the storage of plutonium within the 3,013 canisters.

Pacific Northwest National Laboratory also continues to provide key support for the Spent Nuclear Fuel Project at Hanford including fuel behavior studies and uranium chemistry evaluations to confirm the safety basis that facilitates optimization of drying operations. We continue to provide helium gas purity analysis and are working with the contractor to identify and resolve key safety parameters for sludge packaging and storage.

DOE and the contractors have recently identified plans to expedite the disposition of the cesium/strontium capsules by placing them in dry storage. It is planned that in support of DOE and the on-site contractors, Pacific Northwest National Laboratory will be fully engaged in technical feasibility studies to



a) Before and after Scanning Electron Microscope photos show the reduction of uranium following thermal stabilization; b) Nondestructive Evaluation system developed to measure contamination levels on walls of K-Basins; c) Scaled testing of a new process to precipitate plutonium from solutions; d) Cutaway of an advanced, wireless canister monitoring system for long-term storage of plutonium.

support the accelerated disposition of this high-risk material including the development of safety basis data necessary to confirm cask design.

For DOE-NA-26, the Laboratory is using the Radiochemical Processing Laboratory, a Category II nuclear facility that it manages for DOE, to provide the long-term performance behavior for immobilized plutonium waste forms to support geologic repository disposal. Pacific Northwest National Laboratory is providing technical and contractual support to DOE for the regulatory infrastructure within the Russian Federation to help them meet their disposition requirements in accordance with the bilateral plutonium disposition agreement. The Laboratory is a key team member for establishing the monitoring and inspection technical approach for ensuring compliance with disposition requirements for both the domestic and Russian disposition efforts.

Also, through Battelle's 1831 contract with DOE, Laboratory staff are supporting Washington Group International, Inc. in the design of the Pit Disassembly and Conversion Facility. This facility, to be located at the Savannah River Site, will dismantle classified shapes of nuclear weapons components to support the plutonium disposition program. Pacific Northwest National Laboratory staff are providing key plutonium technology, classification, and environmental safety and health expertise.

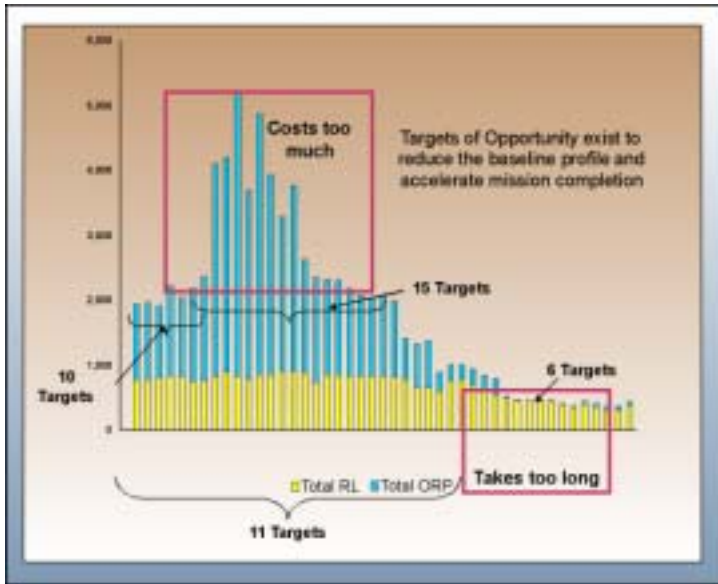
The Laboratory supports DOE-NE-40 mission objectives to develop new or improved radioisotope products and services that are widely used in the U.S. and internationally for medicine, industry, and scientific research. The facilities, scientific expertise, and technical capabilities of the Radiochemical Processing Laboratory support our radioisotopes program. This program focuses on isotope production from generator systems and irradiated targets, recovery and recycle of orphan radioisotope sources, advanced radiochemical separations research, and new radioactive drug and device design and testing. We produce yttrium-90, bismuth-212, bismuth-213, actinium-225, and radium-223 as medical isotopes, and we produce sealed-source cesium-137, cobalt-60, and strontium-90 for industrial and national security needs. We seek to be viewed by government, academia, and industry as an essential national resource for radioisotopes and radioisotope products.

4.2.1.9 Manage Future Risk

The DOE Office of Environmental Management has instituted an accelerated complex-wide cleanup program to achieve more timely progress with cleanup at reduced costs. This will be accomplished by prioritizing cleanup investments according to the extent of risk reduction (human and ecological). At Hanford, DOE has instituted a twofold strategy whereby 1) many sites located along the Columbia River corridor will be cleaned up and ultimately released to the public (reducing DOE's footprint) and 2) Central Plateau sites (primarily the 200 Areas) will be managed as a consolidated waste management complex with many wastes left in place but isolated from the accessible environment.

Pacific Northwest National Laboratory is a key partner in the Hanford cleanup. In addition to our science and technology contributions, we provided the leadership to establish a collaborative partnership between DOE, the regulators, the contractors, the State of Washington, and Hanford's stakeholders. Our

Pacific Northwest National Laboratory is supporting the international plutonium disposition program for DOE-NA-26, the Office of Fissile Materials Disposition, as well as the Hanford interim stabilization program for nuclear material.



This chart shows a view of the Hanford Site cleanup baseline. Pacific Northwest National Laboratory's work with DOE resulted in the identification of areas of the baseline budget where costs can be reduced and schedule can be compressed (see the red boxes).

knowledge of the nuclear processes, the environment, and human health enables us to provide the technical analyses needed to catalyze innovative decisions on cleanup. The result has been a groundbreaking dialogue focused on understanding the barriers and constraints and how these constraints can be eliminated so more rapid cleanup can occur at the Hanford Site that is protective of human health and the environment. We will continue to enable this partnership through our technical analyses.

The Laboratory performs environmental monitoring at Hanford and conducts research supporting the containment and safeguard of hazardous and radioactive materials from the public. This work plays an essential role to our support of the environmental quality mission and aligns our capabilities to advance stewardship of non-free release sites and facilities that DOE will either turn over to others or for which it will retain oversight.

Key research activities that support managing the future risk of the Hanford Site include

- caps and covers to isolate wastes in place
- subsurface reactive barriers to mitigate contaminant migration in the groundwater and vadose zone (e.g., In Situ Redox Manipulation)
- sensors to monitor the migration, attenuation, and eco-toxicity of contaminants (e.g., biomarkers)
- fundamental research dealing with the fate and transport of contaminants in the environment (bioremediation, natural attenuation, etc.)
- risk-based methodologies for the design of environmental monitoring programs
- risk-based decision support tools to optimize Hanford cleanup (e.g., the systems assessment capability).

In conjunction with the Central Plateau strategy, we envision that final closure plans will use surface barriers and subsurface containment systems. We will provide the necessary support to develop these systems and evaluate the performance data necessary for regulatory and stakeholders support for planned Records of Decision at the Hanford Site. We will continue to enhance the barrier design elements and associated monitoring systems to increase effectiveness and reduce costs. Barrier monitoring systems are essential to this technology, as they must have sensitivity and selectivity to monitor slowly changing conditions, be durable during deep remote operation in corrosive environments, and be reliable for long-term operation.

Pacific Northwest National Laboratory also will continue to deliver high-quality science and technology to the Hanford Public Safety and Resource Protection and the Hanford Groundwater Monitoring Project. Our efforts will be directed at developing new environmental monitoring technologies that advance our

capability to understand the impacts of Hanford operations on the environment and the public. For example, new monitoring technologies (e.g., biomarkers) will be developed that focus on novel indicators of chemical-induced stress acting on biota populations (this technique is based upon the induced changes in biological systems as indicated by nucleic acid signatures). Current monitoring approaches will be enhanced to reduce labor-intensive and costly analyses of water samples and ecological systems, and guidelines will be established that can predict the combined toxicity of most mixtures.

The Laboratory will develop the monitoring capabilities required for cost-effective stewardship of residual wastes present at DOE sites, targeting ecological resources rather than the chemical inventory itself. Ecological protection is a primary goal of DOE stewardship, and is a main factor for cleanup of Hanford lands that will be transitioned in the Hanford Reach National Monument.

4.2.1.10 Minimize Waste Generation

Pacific Northwest National Laboratory, through its internal Pollution Prevention Program, is dedicated to helping staff prevent or minimize all pollutants (nonhazardous, hazardous, radioactive) to all media (air emissions, liquid effluents, and solid waste). We are a recognized leader in implementing innovative programs for waste stream minimization, pollution prevention, and resource recycling. In addition to preventing or minimizing waste, we also practice resource conservation, recycling, energy efficiency, water conservation, and purchasing environmentally preferable products and services. Our Pollution Prevention Program provides a wide range of pollution prevention services, including compliance aspects of pollution prevention, such as reporting progress to regulatory agencies.

4.2.1.11 Stewardship, Public Safety, and Resource Protection

The presence of post-cleanup residual contamination at weapons complex sites means that DOE will continue a long-term site management and resource protection program. DOE wants to avoid, delay, or reduce the frequency or impact of harmful exposures to hazardous substances that remain after cleanup projects and other operations are completed. These mitigating efforts will be an Office of Environmental Management priority as sites are cleaned up and made available for alternative uses. Pacific Northwest National Laboratory is supporting the enhancement of DOE's resource protection program on a number of levels. We are participating in Hanford Site resource protection efforts by supporting the development of the DOE Richland Operations Office planning document, The Hanford Long-Term Stewardship Plan: Integrated Long-Range Planning for the



The Public Safety and Resource Protection Program safeguards the public, Hanford Site workers, and ecological and cultural resources through the cumulative assessment of onsite and offsite impacts of site operations.

Site, and planning activities for DOE-Headquarters' National Long Term Stewardship Program. Linking the local and national efforts is our established role in long-term environmental monitoring, ecosystem monitoring, cultural resource management, and risk assessment capabilities. This expertise is providing valuable baseline information to support decisions related to resource management, public safety, comprehensive land use planning, and Site landlord transition efforts and land release.

We are teaming with the Idaho National Engineering and Environmental Laboratory in the development of the National Science and Technology Roadmap. This roadmap will support identification of the DOE complex-wide science and technology needs in the context of development of a resource protection and stewardship science and technology roadmap. This effort is designed to assist in identification and resolution of complex-wide solutions common to stewardship of multiple DOE sites, especially where fate and transport of contaminants and performance monitoring will be ongoing activities.

4.2.2 Capability Development: Role of Laboratory Initiatives

Laboratory initiatives strengthen the environmental science and technology capabilities needed to carry out the above activities. In particular:

- The Biomolecular Systems initiative will provide a better understanding of the relationships between exposure and response—particularly at the cellular level. Research in this area will support our effort to strengthen cleanup policy and will provide stronger risk-based approaches.
- The Computational Sciences and Engineering initiative will develop the science-based capability to optimize new-generation contaminant cleanup technologies and to predict chemical and microbial processes in the subsurface. We are building the technical capabilities and tools that we need to better predict the fate and transport of contaminants through the subsurface.
- The Nanoscience and Nanotechnology initiative will support science to develop novel, more effective chemical separations and will strengthen our ability to provide solutions to the most difficult cleanup problems.
- The Advanced Nuclear Science and Technology initiative will provide novel solutions for environmental remedial action and cleanup of radionuclide-contaminated lands, with focus on special problems in actinide chemistry.

4.2.3 Major Research and Development Thrusts

We are carrying out three major technical efforts to expand our role in the DOE environmental quality research portfolio.

4.2.3.1 Process Science and Technology for Complex Wastes

Pacific Northwest National Laboratory will continue to provide strong process science and technology capabilities to address DOE needs, with special emphasis on complex and special wastes. Strategic advancements in science and targeted technology solutions for addressing these complex special wastes, such as those present in the Hanford high-level waste tanks, will provide cost savings for cleanup.

We will continue to develop work-plan roadmaps and flowsheets that provide critical information on how process systems for Hanford waste treatment perform, so that essential changes can be made before waste treatment begins. We will continue our research efforts on advanced analytical tools and robotic characterization systems for the retrieval and treatment of tank waste streams. We will study the behavior of colloidal agglomerates in tank sludge based on the chemical and physical attributes of solid and liquid phases, and predict their impact on waste processing by simulating simultaneous mixing, dissolution, and precipitation using computational tools such as TEMPEST combined with GMIN. We will conduct experiments to better understand and identify the chemical conditions that control the formation and agglomeration of colloidal and other important particles in waste, allowing for the development of methods to manipulate the waste to optimize tank waste transfer and processing conditions. We will also continue our studies of the behavior of complex tank wastes as they are mixed and treated in preparation for vitrification, and studies of their behavior during the ensuing vitrification process, including calcification of slurries that occurs in glass melters.

4.2.3.2 Environmental and Human Health

We will leverage our 50 years of experience in radiation measurements and dose assessments and will extend worker protection research to areas of increasing interest, such as chemical exposure. Our research will focus on chemical exposure instrumentation and biomarkers. We will develop models that integrate exposure data to predict the biological effects of exposure at the molecular, cellular, tissue, organ, and whole organism levels. We are currently analyzing the DNA damage due to low-dose radiation with a teaming approach that links applied and basic researchers together. We will develop and deliver worker protection technology such as the Pit Viper system that minimizes worker exposure to tank wastes during monitoring and retrieval. Recent legislation requires the federal government to compensate workers who received exposures during DOE's production mission. Our researchers will be involved in reviewing records and determining doses for this program. We are researching brachytherapy techniques and extending our measurement and assessment research into patient safety.

4.2.3.3 Subsurface and Ecological Science

Progress in subsurface science will support DOE in environmental cleanup and stewardship of DOE sites after cleanup. The increased knowledge from subsurface and environmental science research will provide the scientific basis for credible and defensible cleanup decisions and will enable effective environmental remediation at DOE's highest priority sites. We also will develop the scientific and technological bases for conducting routine, cost-effective monitoring of aquatic ecological systems at risk from residual contaminants in groundwater and surface waters of DOE lands. Innovative monitoring capabilities will be developed that focus on novel indicators of chemical-induced stress acting on target populations, and on indicators of changes in community structure that result from chemical-induced stress. We will also develop innovative techniques for tank leak detection, monitoring and mitigation using partitioning tracers, and an understanding of subsurface flow fields.

The computing power in the Environmental Molecular Sciences Laboratory has enabled us to parallelize and improve our modeling codes.

4.3 Energy Resources

Our nation faces acute challenges in the production of sufficient energy to drive our growing economy. The challenges relate both to diminishing natural resources and to an aging and inadequate energy infrastructure. Pacific Northwest National Laboratory is engaged in research and technology development that will benefit DOE's energy mission by providing insight and technology in five areas where we can deliver added value: clean and efficient vehicles, efficient buildings systems technology, efficient and economical power technology, clean and productive industries, and advanced science and technology for nuclear energy.

4.3.1 Strategic Intent

We will focus the resources of the Laboratory—from basic research to engineering development—to create valuable solutions that impact the ability of U.S. industry to respond to the Department of Energy's mission objectives and national energy needs. The Laboratory will seek to accomplish these outcomes through effective collaboration with industry and other national laboratories and by building on our long history of collaborative industrial research.

Pacific Northwest National Laboratory's capabilities in materials science, fuel cell technology, energy transmission and distribution, sensors and controls, systems engineering, computational engineering, manufacturing process innovation, nuclear engineering and nuclear materials process engineering will be used to demonstrate new technology important to DOE's strategic energy goals. We will maintain our technical strengths in building codes and standards and will greatly increase the scientific and technical content of our energy programs in advanced power and transportation systems, industrial efficiency, climate-change issues, and

electric power distribution and transmission technology. We also will build on the Laboratory's strengths in fundamental materials science to develop novel optical and electronic materials, new high-temperature materials for advanced fuel cell systems, and we will advance our knowledge of radiation-induced damage to metals and ceramics leading to important new materials for nuclear applications.

Supporting our strategy for innovation, we are investing internal resources in technical thrust areas of fuel cell systems technology, power generation and transmission technology, efficient and lightweight vehicle structures, emissions-reduction technology, and advanced technologies for nuclear energy applications. Through these investments, the Laboratory will provide leadership and accomplishment to DOE's energy resources agenda.

We will support energy resources in developing robust strategies that address the technological implications and market impacts of carbon management. This will be accomplished by focused investments in bio-derived fuels and feedstock products. Each element of our



Researchers at the Pacific Northwest National Laboratory are working to solve the technical challenges required for the widespread use of fuel cells in vehicles and other applications.

energy resource strategy is integrated into a crosscutting carbon management agenda. We are providing a balanced perspective to the technological, ecological, and economic dimensions associated with stabilizing and reducing atmospheric carbon levels.

4.3.2 Our Role in the Energy Resources Research and Development Portfolio

Pacific Northwest National Laboratory will advance DOE's mission to provide efficient and productive energy use and clean and affordable power by contributing to the high-level objectives defined in the energy resources research and development portfolio. We will strive to develop new technologies in each of the major focus areas of the portfolio: reliable and diverse energy supply, clean and affordable power, and efficient and productive energy use. Specifically, research in energy science and technology at the Laboratory will focus on advanced fuel cell technology, the development of cleaner and more efficient heavy vehicles, energy-efficient buildings and building-support systems, advanced nuclear science and engineering, and new technologies for helping industry reduce manufacturing costs and increase the energy efficiency of energy-intensive processes. We are developing an integrated approach to distributed generation of electric power that couples the supporting information and control infrastructure necessary to establish distributed generation as an economically viable option for utilities, industry, and the consumer.

4.3.2.1 Efficient and Productive Energy Use

Automobiles, trucks, buildings, and industries are major consumers of energy resources. Pacific Northwest National Laboratory is engaged in research to meet current and future energy consumption challenges.

Clean and Efficient Vehicles

We will continue to develop lightweight materials and new manufacturing technologies that support vehicle fuel mileage reduction in light and heavy vehicles. We will develop new fuel cell technologies for auxiliary power sources and hybrid propulsion systems, cleaner fuels, and more effective advanced vehicle emission reduction technologies that will be key to DOE's new FreedomCAR Program.

Our leadership in the Northwest Alliance for Transportation Technologies highlights our role in achieving clean and efficient vehicles. These efforts are coordinated with the 21st Century Truck Program, a new multiagency partnership focused on improving the performance of trucks. These are public-private partnerships designed to meet the challenges of developing automobiles and trucks with reduced pollutant emissions and higher fuel efficiencies. The Northwest Alliance has positioned Pacific Northwest National Laboratory as a player in mission-critical areas for automotive and heavy-vehicle manufacturing.

The strategic foundation of the Alliance is to establish a systems management approach that links our technical competencies in advanced energy systems, materials innovation,



Pacific Northwest National Laboratory is providing leadership to the Northwest Alliance for Transportation Technologies and the 21st Century Truck Program to meet the challenge of increasing fuel efficiency and reducing vehicle emissions.

virtual system simulation, and manufacturing process innovation. This linkage and critical outcome drives the FreedomCAR and 21st Century Truck programs, as well as other DOE programs for clean, energy-efficient heavy vehicles. Strategic alliances developed with the automotive and heavy-truck industries will ensure that industry needs are met, and that commercially viable technology and intellectual property is readily transferred and adopted by the auto and heavy-vehicle industries. Our initiatives also develop new capabilities in vehicle emission reduction technologies, vehicle power systems, and advanced lightweight materials.

Industry needs new engineering simulation and design tools if new materials and manufacturing processes are to be adopted. Building on Pacific Northwest National Laboratory's strengths in large-scale, high-speed scientific computing and simulation, we are aggressively pursuing new approaches to engineering simulation tools and approaches that use the capabilities of massively parallel supercomputers. These engineering simulation efforts are integrated within the Laboratory's Computational Sciences and Engineering group.

Efficient and Affordable Buildings

In addition to providing a place to work and live for nearly all Americans, our buildings must provide a healthy and safe indoor environment. In addressing this need, Pacific Northwest National Laboratory focuses on multidisciplinary solutions to improve building energy efficiency. We also are looking closely at ways to improve the comfort and health of building occupants.

The Laboratory supports the initiation of the Buildings of the 21st Century program that will integrate modern building technologies. We are an established leader in developing automated diagnostics for building applications. We played a critical role in developing and implementing model energy codes and standards. We team with the building industry and with other partners to improve the energy efficiency of the buildings and to increase their use of renewable resources. We currently work with industry to develop intelligent building capabilities such as microscale heat pump concepts for building temperature control.

Clean and Productive Industries

Inefficient industrial processes use vast amounts of energy and frequently have unwanted environmental impacts. Pacific Northwest National Laboratory's support to the clean and productive industries mission covers a broad range of activities, from program planning and technical evaluation to technology development and demonstration. For example, the Laboratory is developing new technologies and computational tools for simulating manufacturing processes in glass, metals, and composites. These new tools are designed to accelerate innovation while reducing development and production costs. We also are studying alternative bio-derived fuels and bio-derived chemical feedstocks for the industrial chemical sector.

Our process science and engineering competencies develop new methods for recovering energy from industrial and agricultural waste, identifying renewable routes for value-added chemical manufacture, and enhancing pulp and paper plant efficiencies with improved



Scientists at the Pacific Northwest National Laboratory are taking biomass conversion processes from the laboratory to industrial applications.

separation technologies. We are applying our capabilities in sensors and advanced manufacturing to glass fabrication through the use of noncontact stress measurement techniques and advanced process control methods. Other novel sensors will help the pulp and paper industry to measure pulp slurry characteristics and paper web properties.

The Laboratory also provides leadership for the Industries of the Future Laboratory Coordinating Council. This group facilitates access to Laboratory capabilities that can help solve major technology challenges. One of our collaborations with other national laboratories, industries, and universities uses advanced computations and modeling to address a key issue of chemical plants—the characterization of multiphase fluid dynamic behavior.

4.3.2.2 Clean and Affordable Power

Advanced energy technologies can provide abundant power without the emission of harmful contaminants. Pacific Northwest National Laboratory is developing technologies to overcome many of the immense technical obstacles that limit the broader application of such systems as clean and affordable energy sources for our nation.

Work related to distributed and hybrid systems, which includes renewable technologies and fuel cell technology, continues to expand in recognition of potential environmental benefits and advantages of increasing distributed generating capacity.

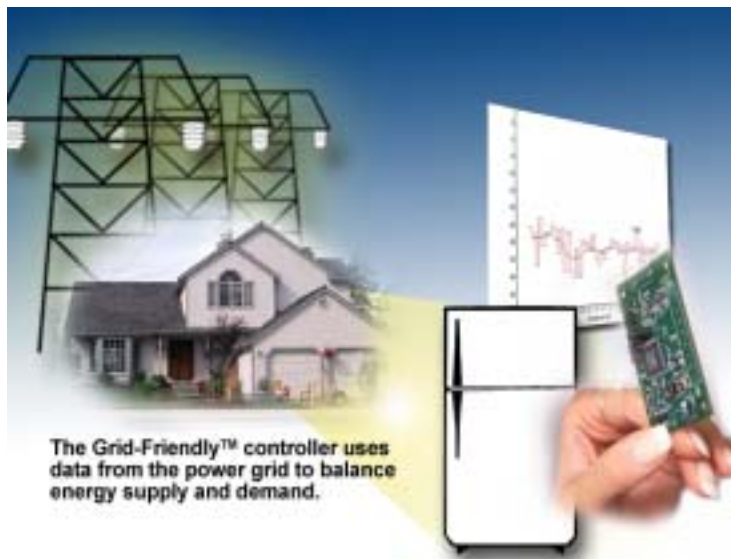
In the future, advanced coal and natural gas-fueled power technologies must provide high efficiency and low emissions, with eventual integration into power plants to achieve even higher efficiency, provide greater fuel flexibility, reduced or net-zero emissions, and generate power at lower cost. Fuel cell technology will play a central role in Pacific Northwest National Laboratory's advanced energy systems thrust, and carbon sequestration will become an increasingly important option for coping with greenhouse gas emissions. The Laboratory will help to build and lead new government/industry partnerships in testing and demonstrating carbon capture and sequestration technology.

Efforts on advanced nuclear technology are focusing on helping to ensure that nuclear plants can deliver affordable power beyond their initial license periods, the development of new materials for reactor designs that offer improved economics, processing technologies that reduce waste generation, and nuclear engineering expertise that increases safety and proliferation resistance.

Advanced Power Systems

Our efforts in solid oxide fuel cell technology center around a program called the Solid-State Energy Conversion Alliance jointly managed with the National Energy Technology Laboratory. This public-private alliance between federal agencies that fund advanced fuel cell research targets the transportation, mobile-military power, and stationary-power markets. The members of this alliance share a common commitment to commercializing cost-competitive, high-efficiency, fuel cell power.

As the ultraclean fuel cell technology advances to widespread use in stationary-power and transportation applications, the high efficiency inherent in these technologies will result in reduced carbon dioxide emissions and lower costs for



power. The alliance approach coordinates federal research and development investments and program integration as well as encouraging leveraged industrial investments.

As the nation begins to develop and adopt the next generation of power systems, carbon capture and carbon sequestration technology will need to be developed for low or net-zero carbon emissions systems. Critical in the development of these technologies will be new government/industry partnerships for the demonstration and testing of commercial scale zero-emission technologies. Pacific Northwest National Laboratory is an active participant with DOE in developing technology roadmaps and consensus opinion with the national large power producers relative to carbon capture and carbon sequestration strategies.

Enhancing the Utility Infrastructure

Inefficient energy grids waste electrical power and increase the costs to consumers. Pacific Northwest National Laboratory has extensive experience working with DOE and the utility industry to address the technology needs for reliable electricity supplies in the 21st century. Laboratory staff conduct research to improve the operation and maintenance of power utility infrastructure and power-distribution control. We provide technology for reliable control of power plants, wide-area monitoring of utility grids, frameworks to facilitate deployment of distributed resources, and infrastructure security. We have established partnerships with the utility industry on distributed resource systems and policy studies, grid reliability technology research, and new intelligent system control frameworks. The Laboratory will continue to collaborate with federal energy agencies on potential energy test beds and demonstrations.

Pacific Northwest National Laboratory has developed a real-time power system control called the Wide-Area Measurement System that aids in analyzing utility grid reliability. We conduct programs in energy resources management, environmental impact studies, and market transformation, which serve the power and energy services entities. We will be supporting the new initiatives in grid reliability and distributed resources. We will seek to deliver advanced operations and maintenance technologies to the power and transmission entities to aid in reducing regional power costs.

4.3.3 Major Research and Development Thrusts

To develop and expand our contributions to the energy resources research and development portfolio, Pacific Northwest National Laboratory is pursuing the following thrust areas:

- **Fuel Cell Technology Development**—This program will overcome barriers to mass customization of solid oxide fuel cell technology. This research focuses on developing high-temperature materials, novel designs for planar solid oxide

fuel cells, improved manufacturing processes, catalytic fuel reformation systems, computational engineering and systems simulation, diagnostics, and control systems.

- **Lightweight Materials for Transportation Applications**—This program improves Laboratory competencies in system design, materials innovation, virtual system simulation, and manufacturing process innovation. Our goal is to produce improved light metal alloys and composites and to deploy these new materials in automotive and heavy vehicle structures.
- **Compression-Ignition Direct-Injection Emissions Reduction Technology**—This program is aimed at developing advanced diesel emissions technology needed for the industry to comply with mandated emission standards that are to be phased in during the decade. Our goal is to develop accurate physical models for the entire combustion and exhaust systems, new catalytic materials for after treatment, and new methods for the reduction of particulates and sulfur.
- **Energy Networks**—This program provides the leadership and technology required to simulate and operate the complex network represented by the nation's future electric power infrastructure. This new network will rely heavily on information technology for monitoring, control, and operations. Research at the Laboratory focuses on the mathematics required to model the underlying supply and demand network and the creation of software required to simulate, operate, and control the network and its subcomponents in a secure manner.



Our expertise in materials science and advanced manufacturing techniques allows us to focus on developing new lighter weight materials for transportation that also are economical to manufacture.

- **Bio-Based Products**—This initiative builds an integrated portfolio of capabilities in biological, chemical, and supporting process science technology. The initiative supports DOE's efforts to produce chemicals, fuels, materials, and power from domestic sources; reducing our dependence on foreign oil.
- **Advanced Instrumentation and Controls**—This program focuses on developing intelligent diagnostic systems for on-line monitoring of plant equipment using, for example, smart sensors and Decision Support for Operations and Maintenance (DSOM® - R&D 100 Award, 2000).

4.3.4 Capability Development: Role of Laboratory Initiatives

Our energy sciences and technology initiatives strengthen the Laboratory capabilities that are needed to carry out the major DOE research and development objectives.

Homeland security – protection of the United States and its assets – is and will be a national priority for the foreseeable future.

- Pacific Northwest National Laboratory's Fuel Cell Technology initiative extends the Laboratory's capabilities in materials chemistry and ceramics into a broader set of capabilities in the development of solid oxide fuel cell systems. Our goals are to develop robust component materials and new planar solid oxide fuel cell designs, as well as to establish the manufacturing methods that will enable the mass production of the technology.
- Our Computational Sciences and Engineering initiative builds capabilities and tools for virtual manufacturing software applications, including material property studies, advanced fluid dynamics tools for fuel cell designs, advanced engineering mechanics, problem-solving, and a broad range of simulation capabilities associated with engineered systems.
- Our Carbon Management initiative builds on Laboratory expertise in climate research. This initiative will support DOE with technologies for limiting carbon releases to the atmosphere. The Laboratory is conducting basic research on specific carbon management technologies (such as low-carbon fuels, bioenergy, and carbon sequestration technologies) that are novel and that are identified as critical to solving the climate change problem.
- Our Advanced Nuclear Science and Technology initiative refocuses and reinvigorates the Laboratory's strengths in key technology areas (e.g., nuclear materials) relevant to the development of next-generation nuclear energy systems as one component of an integrated strategy for meeting the nation's future energy needs.
- The goal of the Energy Systems Transformation initiative is to research, develop, and deploy a new generation of technologies for the nation's energy infrastructure. The advent of distributed and embedded digital intelligence in virtually all devices, at low cost, offers the opportunity to transform the energy systems.

4.4 National Security

The 21st century threats to national security have never been more potentially devastating to countless U.S. citizens and our national interests—both at home and abroad. Proliferation of weapons of mass destruction and their associated delivery systems remains a worldwide concern. There is an increasing awareness of the potential for unconventional (biological, chemical, nuclear, radiological, and cyber) threats to the United States and its assets abroad. The events of September 11, 2001, and our government's response, continue to dramatically highlight and reshape national security mission priorities and supporting research and development programs. Terrorism, and the impact on American citizens within our homeland borders, presents challenges of dimensions never before faced by our government and security operations. The continental United States is no longer recognized as a sanctuary, major shortfalls in U.S. intelligence operations have been highlighted, and the U.S. military faces unprecedented challenges to transform forces, equipment, and organization in order to meet new mission requirements. The Department of Energy and its national laboratories have a critical role in addressing these national security issues by providing leadership and technical solutions in support of national policy.

4.4.1 Strategic Intent

The Laboratory's national security mission is to develop and deploy innovative solutions to critical national security challenges. Our primary focus is to effectively and responsively support DOE clients who promote the security interests of the United States. However, in so doing, and in concert with our primary DOE sponsors, our national security research and development portfolio extends into other government and private organizations with complementary national security mission requirements.

The Secretary of Energy has outlined his vision for DOE having an overarching mission of national security. He emphasized the critical importance of national security-related research and development as the underpinning and focus of the entire department. At Pacific Northwest National Laboratory, our response to the Secretary's vision is clear and straightforward—we will employ the Laboratory's significant science and technology capabilities to develop and deploy innovative solutions to critical national security challenges.

4.4.2 National Security Clients

The Laboratory's national security work is conducted for several DOE organizations. Our principal client is the National Nuclear Security Administration (NNSA), with the Office of Defense Nuclear Nonproliferation and Defense Programs being the primary focus. Other important DOE clients include the Office of Counterintelligence, Office of Intelligence, Office of Security, and Office of Emergency Operations.

On a broader scope, DOE and this Laboratory also play an essential role in providing technical expertise and innovative science-based solutions to other organizations having a national security mission. The Department of Defense; the State Department; the Department of Justice; the Federal Bureau of Investigation; federal, state, and local law enforcement organizations; the new Department of Homeland Security; and many counterterrorist organizations are examples of these clients whose needs we serve through the Work for Others program. This program is outlined in more detail in Appendix A, Work for Others.

4.4.3 Our Role in the DOE National Security Research and Development Portfolio

This report describes selected Laboratory research and development programs and technical contributions for each of our key clients within DOE. Program descriptions for each client are organized around the national security research and development portfolio as it was defined by DOE in 1997 in five portfolio areas: 1) maintaining the nuclear deterrent, 2) monitoring nuclear treaties and agreements, 3) preventing proliferation, 4) detecting proliferation, and 5) countering weapons of mass destruction terrorism.

4.4.3.1 National Nuclear Security Administration (DOE-NA20)

The National Nuclear Security Administration faces key challenges in responding to evolving requirements in nuclear deterrence, arms reduction, and nonproliferation R&D. Following is a description of selected research and development programmatic support to the NA-20 mission needs.

BEADS, short for Biodetection Enabling Analyte Delivery System, is a sample preparation system that concentrates large volumes of environmental samples into small, clean samples that can be used in biodetectors to quickly identify pathogens.

Monitoring Nuclear Treaties and Agreements

Nuclear Explosion Monitoring. For greater than half a century, Pacific Northwest National Laboratory scientists and their Hanford Site predecessors have been global leaders in monitoring man-made sources of radioactivity in the environment. Throughout the Cold War, the Laboratory operated sensitive systems for analyzing fallout and other samples from nuclear tests. In recent years the Laboratory has increased its technical, policy, and program leadership support to the National Nuclear Security Administration's need for development and deployment of innovative technologies for international arms control and nonproliferation efforts. The Laboratory's nuclear explosion monitoring program is an excellent example of this increased commitment and focus where we bring Laboratory scientific and engineering expertise to bear on the technical and policy challenges of monitoring nuclear treaties and agreements. The following examples illustrate the Laboratory's support to NNSA's nuclear explosion monitoring program.

- Providing enhanced radionuclide collection and analysis capabilities needed to monitor other nations' compliance with nuclear explosion monitoring agreements and to satisfy its monitoring obligations as established. To do this, we develop, transfer, support, and enhance the necessary radionuclide technology needed for fully automated remotely programmable systems that monitor atmospheric concentrations of radioactive particles and noble gases with exceptional sensitivity for near real-time measurements.
- Providing staff expertise to assist in negotiating cost-effective nuclear explosion monitoring agreement implementation measures. To do this, we send radionuclide experts to interagency meetings to advise on technical policy, and we provide radionuclide experts to staff the U.S. delegation.
- Providing statistical tools and expertise needed for optimum processing and interpretation of nuclear test monitoring data. When attempting to detect and characterize extremely weak signatures, as is necessary when using a few stations for monitoring the entire globe, it is easy to confuse signals and noise or other irrelevant phenomena. For this reason, statistical methods are designed carefully and applied to enhance the reliability of interpretations. This is accomplished by cooperating with seismic experts at other institutions to optimize processing and interpretation of waveform data and by developing new statistical tools to minimize the costs of operating monitoring capabilities.

Nuclear Nonproliferation and Arms Reduction Monitoring. DOE has a critical role in the Administration's interagency-wide effort to reduce the number of nuclear weapons and the amount of weapons-grade material both in the United States and in the former Soviet Union. Technology must be developed, demonstrated, and deployed for confirming that an examined object is a nuclear weapon or a weapon component, without releasing any nuclear weapons design information or other information deemed sensitive by either the United States or Russia. Nuclear materials must be monitored in long-term storage to maintain security until proper disposition.

Pacific Northwest National Laboratory is a key participant in DOE's efforts to develop technology that will verify the presence of nuclear material in a warhead, or that nuclear material was derived from a nuclear weapon, yet also have robust information barriers that prevent disclosure of classified or sensitive information. We also provide technical support to DOE and other policymakers regarding

START III negotiation options. We also participate in United States/Russian technical exchanges on very sensitive topics under the Warhead Safety and Security Exchange agreement.

Preventing Proliferation

Arms control treaties and agreements have resulted in significant amounts of weapons-usable fissile materials becoming excess to national defense needs in both the United States and Former Soviet Union states. Protection of these excess fissile materials from theft and unauthorized uses is of utmost importance. DOE's research and development portfolio for preventing proliferation addresses the following areas:

- developing and implementing technologies that convert U.S. weapons-usable plutonium into forms that prevent its use for nuclear weapons
- assisting Russia in the demonstration of plutonium conversion technologies
- developing technologies to control and account for nuclear materials and physically protect these materials
- developing proliferation-resistant fuel for commercial reactors, to reduce the potential for civilian reactors to generate material that may be reprocessed into nuclear weapons-grade materials
- shutting down the remaining three plutonium production reactors still operating within the Russian Federation while providing replacement heat and power.

The following paragraphs highlight several programs at the Laboratory that contribute to DOE's goal of preventing proliferation.

Fissile Materials Disposition. Pacific Northwest National Laboratory provides leadership, collaborative assistance, and needed technologies in support of the National Nuclear Security Administration's efforts to dispose of weapons-grade fissile materials. Our customers in this important area include DOE, other national laboratories, and prime contractors to DOE-NA-26. Our primary focus with this effort is to integrate science, engineering, policy, and integrated safety management to support the following technology needs:

- direct programmatic support to DOE Headquarters in fields of regulatory analysis, life cycle programmatic planning, and development of monitoring and inspection technologies
- developing technologies to immobilize and dispose of weapons-usable plutonium
- burning weapons plutonium in mixed-oxide fuel in existing domestic reactors
- demonstrating to Russia that plutonium immobilization is a viable disposition option.

Nuclear Materials Protection. Effective material protection, control, and accounting measures will deter suppliers and potential terrorists who seek long-term access to material for diversion. The Laboratory has a lead role in the development of real-time inventory and monitoring technologies for current and



Scientists at the Pacific Northwest National Laboratory are developing an Acoustic Inspection Device that is ideal for identifying concealed objects, such as hazardous materials in closed containers.



Our extensive background in global security dates back to the World War II era – from the development of technologies that will help detect and prevent the use of weapons of mass destruction to helping diversify economies in former Russian nuclear “closed cities.”

future materials protection, control, and accounting requirements. Following are some specific programs and technologies:

- research, development, and evaluation of microsensors, information, and collaborative technologies for rapid inventory and remotely attended monitoring
- physical security and accountancy upgrades at international facilities appropriate for the level of material attractiveness and the threat of theft, and consolidation of nuclear material into fewer buildings and at fewer sites
- conversion of excess weapons-grade highly enriched uranium and low enriched uranium to reduce the number of theft targets
- cooperative programs with Russian Minatom, Navy, and Gosatomnadzor (GAN) officials to foster the capabilities and commitment of sustained nuclear material protection improvements after U.S. active involvement ends

- assessment and tracking of nuclear smuggling and nuclear threat cases
- enhancing international nuclear emergency early warning preparation and response capabilities.

Proliferation Resistant Fuel Cycle Technologies. We support target development and processing for medical isotope production using reduced enrichment research and test reactor fuel.

International Nuclear Safety Program. Pacific Northwest National Laboratory will continue to provide responsive and focused technology and program leadership support to the National Nuclear Security Administration for international nuclear safety and security missions. This important DOE program, one of the largest single funding clients at the Laboratory, reduces the risks coming from Soviet-designed reactors by establishing cooperative programs with host countries to upgrade nuclear power plants to meet international standards and to build lasting safety cultures. An example of the effort is our continued leadership of bilateral efforts to stabilize the deteriorating shelter surrounding the destroyed Chernobyl reactor in Ukraine.

We also will support the transition of nuclear safety programs and technologies from the former Soviet Union to nations with emerging nuclear programs, such as China and Vietnam.

Initiative for Proliferation Prevention. Pacific Northwest National Laboratory participates in the Initiative for Proliferation Prevention with the Newly Independent States of the former Soviet Union. The goals of this U.S. government program, executed jointly by the Department of Energy and the Department of State, are to

- stabilize supporting technology, equipment, and facilities to enhance global nonproliferation

- develop commercial opportunities and markets for advanced technology
- enhance U.S. science and engineering capabilities
- engage weapons scientists, engineers, and technicians in nonweapons-based activities.

Pacific Northwest National Laboratory will continue to provide the majority of laboratory expertise to the chemical and biological cooperative program under the Initiative for Proliferation Prevention.

Nuclear Cities Initiative. The Nuclear Cities Initiative is a joint United States/Russian program designed to improve U.S. security by assisting Russia in enhancing economic opportunities in the Russian closed nuclear cities as they reduce the size of their nuclear weapons complex. The goal is to provide economic stability and reduce the incentive for Russian nuclear scientists and technicians to migrate to other countries of proliferation concern. Pacific Northwest National Laboratory helped establish and provides staff to serve on the Boards of two International Development Centers in Zheleznogorsk and Snezhinsk. These International Development Centers provide critically needed business infrastructure support and business consulting and services to all the citizens of these two cities and have been among the Nuclear Cities Initiatives most visible and successful activities. The Laboratory will continue to leverage its core competency in regional economic development to similar problems in Russian closed nuclear cities.

Detecting Proliferation

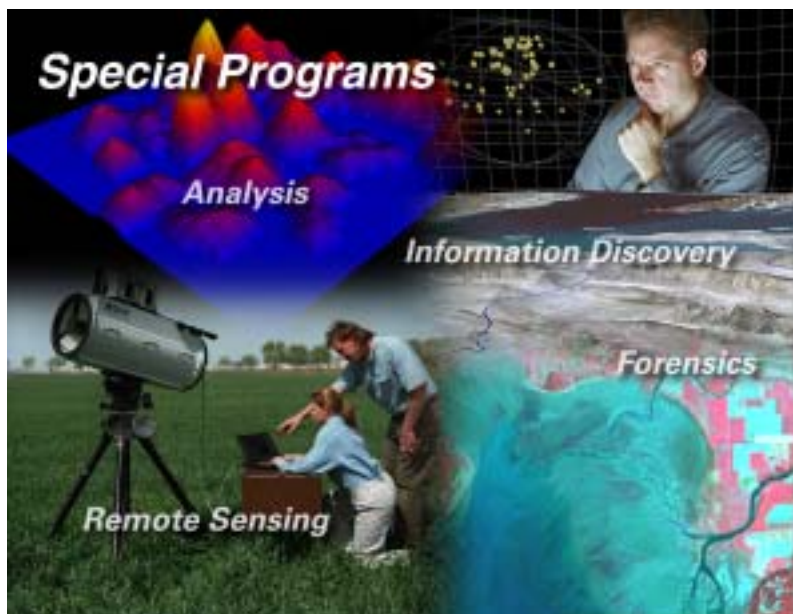
Physical and Chemical Detection. Pacific Northwest National Laboratory develops solutions for a wide array of national security needs dealing with detection and identification of chemical effluents and physical signatures in order to reveal the proliferation or spread of weapons of mass destruction. Many of the effluent and physical detection technologies also have direct civil applications, particularly in environmental applications.

Effluent Detection Technologies. The Laboratory's effluent detection programs include the development and demonstration of sensor systems for detection of chemical signatures that indicate proliferation of weapons of mass destruction. Among the national security needs we addressed are:

- identifying chemical effluents from the production of nuclear, biological, and chemical weapons
- identifying and mapping chemical warfare agents on the battlefield
- assessing battle and collateral damage from strikes against nuclear, biological, and chemical weapons and industrial targets
- supporting counterterrorism activities.

Civilian and research applications of chemical detection systems include counter-narcotics operations, atmospheric chemistry and meteorology, environmental monitoring and cleanup, and industrial and agricultural process control.

Infrared Sensing Technologies. Infrared sensing technology research and development at the Laboratory is focused on detecting the proliferation of nuclear, biological, and chemical weapons using infrared optical sensing technologies that address the need for remote chemical detection. Laboratory infrared sensing



At the Pacific Northwest National Laboratory, our scientists and engineers are the providers of choice for technical analyses, environmental forensics and information science and technology serving the U.S. Intelligence Community.

research also involves multiple science and engineering disciplines in other major areas that include: signatures identification, sensor development, and data exploitation. The Laboratory has profound strengths in a wide array of science, technology, and engineering fields related to infrared sensing developed through Laboratory initiatives. These strengths provide the basis for broader participation in DOE's national security-related remote chemical detection program and related Department of Energy and Department of Defense programs.

Imaging Science and Technologies.

Pacific Northwest National Laboratory will continue to grow its capabilities to provide quality analysis of remote sensing data. Image analysts and investigators in many different applications face common challenges in processing an overwhelming amount of increasingly complex image data. In addition, they must deal with many complex software

analysis packages, each of which provides only a partial solution. Our goal is to become a leading innovator and developer of data analysis algorithms and techniques for exploitation and imaging of remote sensing data.

The Laboratory-level initiative in imaging science and technology is developing capabilities relevant to proliferation detection, treaty verification, and environmental forensics. These scientific discoveries and developments offer significant opportunities beyond national security. With the next generation of imaging tools, analysts and decision makers will have better, faster access to information and greater understanding and insight for solving problems at micro and macro levels. Continued growth in these focus areas will allow the Laboratory to increase its support of the Department of Energy, the Department of Defense, and other government agencies.

Pacific Northwest National Laboratory also conducts applied research and development on remote physical detection analysis for a variety of other clients in addition to DOE. Examples include automated land-use classification, rangeland management, agricultural analysis, and applications in exploration for minerals, oil, and gas.

Future imaging science related technologies being developed by Laboratory staff include enhancing the statistical analysis of data, automating data processing, improving data visualization, knowledge discovery, and creating links to other forms of information technology. These capabilities will enhance our ability to serve the evolving needs of national security clients and help us support new clients in environmental monitoring.

Countering Weapons of Mass Destruction (WMD) Terrorism

Nuclear Weapons. Pacific Northwest National Laboratory will continue to expand its position as a national resource for technologies to counter nuclear

terrorism and reduce the nuclear danger. Our research and development will draw heavily on the Hanford Site experience and core competencies in radiation detection and environmental science and technology. Our major emphasis will continue to be satisfying user needs while advancing the state of the art in measurement sensitivity and selectivity, while minimizing cost.

Countering nuclear terrorism requires specific focus on detection systems, nuclear materials tracking and interception, nuclear materials forensics, and attribution assessment. Laboratory staff will research new technologies to exploit the intrinsic and stimulated radiation signatures of special nuclear materials and to evaluate their performance in various scenarios. Emphasis will be directed toward new, room temperature gamma-ray sensors (such as cadmium-zinc-telluride crystals), advanced low-power digital electronics, highly enriched uranium detection, and cost-effective detector technologies for field applications.

Pacific Northwest National Laboratory will continue to research, develop, and evaluate nuclear materials tracking and tagging technologies that will improve law enforcement and the broader counterterrorism community's capability to respond to diversion of materials. These technologies will support real-time material tracking, material search, near-field pursuit, and infrastructure protection.

Forensic analysis and data interpretation will be developed to identify the sources and illicit routes of seized nuclear materials. The Laboratory will continue to develop rapid in-field forensic technologies and procedures for the attribution assessment of illicit nuclear materials, and extend them to post-event scenarios.

Chemical and Biological Warfare Defense. For many years, Pacific Northwest National Laboratory has supported DOE and other government agencies in chemical detection and remote sensing as applied to chemical effluents from a variety of military and industrial processes. The NNSA Chemical and Biological Nonproliferation Program supports research at the Laboratory on biological signatures and use of the Aerosol Research Facility as a biological agent detector test bed. The Aerosol Research Facility, one of two environmental wind tunnels in the world ideally suited for complex experiments on agent fate, is a significant and unique Laboratory capability that will continue to be applied in support of our defense against chemical and biological weapons.

Laboratory scientists continue to receive recognition from DOE, the Department of Defense, the Federal Bureau of Investigation, and other agencies for work on biological pathogen detection. Laboratory scientists are helping to define the national priorities for protecting the U.S. civilian population against chemically or biologically armed terrorists. Our scientists also are asked to support related efforts by the Centers for Disease Control and Prevention and the National Institutes of Health. We are working with regional public health



Scientists and engineers at the Pacific Northwest National Laboratory are contributing innovative technology solutions and leadership to help transform the military for the 21st century.

services to equip health providers with the ability to prepare for and respond to potential biological agent attacks. We also provide research, development, and analysis to the Department of Defense, the Federal Bureau of Investigation, the State Department, and the intelligence community on chemical/biological weapons defense R&D issues.

The Laboratory's mission in environmental cleanup of former nuclear weapons production activities provides an outstanding base for addressing chemical and biological hazards and mitigation, such as clouds of chemical and biological agents. As a basic science multi-program laboratory, we apply our nuclear materials detection experience directly to applications involving the decontamination and demilitarization of chemical and biological weapons agents and successfully detect, defend against, and mitigate or neutralize attacks on an organization's information and infrastructure functions and systems.

*Pacific Northwest National Laboratory will provide science and technology knowledge and expertise in support of a new National Bureau of Asian Research initiative titled **Tracking the Strategic Environment in Asia.***

International Security and Nonproliferation

Pacific Northwest National Laboratory and the University of Washington have combined to establish the Institute for Global and Regional Security Studies (IGRSS). The three principals are the University of Washington's Jackson School of International Studies, the Department of Political Science, and the Laboratory's Pacific Northwest Center for Global Security. The Institute for Global and Regional Security Studies is intended to promote greater understanding within the Pacific Northwest of issues affecting the national security of the United States, and expand the Laboratory's capacity to serve its DOE client base by providing greater access to the academic community. In its first 18 months, IGRSS has initiated an entirely new academic curriculum on security studies, sponsored colloquia and conferences, and started a new publication series on international security.

The Foundation for Russian American Economic Cooperation (FRAEC) is a strategic Laboratory partner. The FRAEC/Pacific Northwest National Laboratory collaboration dates to the origins of the Nuclear Cities Initiative when the Laboratory recruited FRAEC to serve as a key partner in establishing the International Development Centers in two of Russia's closed nuclear cities. Since this initial collaboration, FRAEC has continued to serve in this capacity under direct contract to DOE. FRAEC continues to work with the Laboratory on other Nuclear Cities projects, including delivery of equipment to the city of Zheleznogorsk, helping the city of Zheleznogorsk on a strategic downsizing plan, and working with the city of Zheleznogorsk to set up a new software development company. FRAEC is a nonprofit organization serving a dual mission of meeting the day-to-day needs of member organizations conducting business in Russia, and on a more global scale, fostering a better business environment in Russia.

The National Bureau of Asian Research and Pacific Northwest National Laboratory have entered into a strategic alliance under the auspices of the Laboratory's Pacific Northwest Center for Global Security. The *Strategic Environment* 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 the sponsorship of Pacific Northwest National Laboratory, 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. The National Bureau of Asian Research is a nonprofit, nonpartisan institution

that conducts advanced research on policy-relevant issues in Asia. It also serves as the global clearinghouse for Asian research conducted by specialists and institutions worldwide.

Under the direction of George Russell, the former president of the Frank Russell Company and Chairman of The Russell Family Foundation, Pacific Northwest National Laboratory has received assistance on Russian economic matters related to our fostering of a worldwide initiative to swap Soviet-era Russian Federation debt for programs on nonproliferation. The products of this strategic relationship resulted in the unanimous passage by the United States Senate of the Debt-Reduction-for-Nonproliferation Act of 2001, an authorization bill cosponsored by Senators Joe Biden and Richard Lugar. At this writing, the Bush Administration also is considering a similar agenda item for discussion with European and Russian counterparts. This work also was a result of a partnership formed with the Nuclear Threat Initiative, having Ted Turner as its benefactor and co-chair with Senator Sam Nunn. The Nuclear Threat Initiative provided funding to Battelle's Pacific Northwest Division to study the implementation of a Russian nonproliferation debt fund.

Princeton University and the University of California at Los Angeles contribute their expertise to our research on micro-electromechanical and nano-lithography technology, and to our development of micro-laser transmitter arrays for infrared chemical sensing. We also collaborate with the University of Idaho to develop methods for detecting trace chemical vapors by infrared absorption spectroscopy. The Laboratory also collaborates with Washington State University on studies of cadmium zinc telluride, a semiconductor material used in solid-state gamma-ray spectrometers. These technologies are important for nuclear arms control, nonproliferation, and verification activities vital to national security.

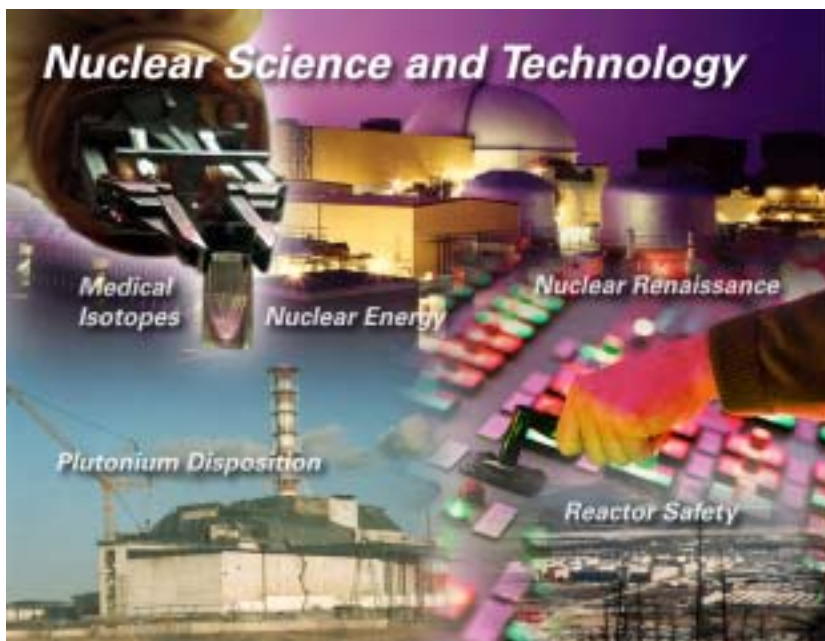
4.4.3.2 National Nuclear Security Administration Defense Programs (NA-10)

Maintaining the Nuclear Deterrent

The Deputy Administrator for Defense Programs within the National Nuclear Security Administration is responsible for achieving national security objectives established by the President for nuclear weapons and assisting in reducing the global nuclear danger by planning for and maintaining a safe, secure, and reliable stockpile of nuclear weapons and associated materials, capabilities, and technologies in a safe, environmentally sound, and cost-effective manner.

The Laboratory will continue to support DOE's Office of Defense Programs in areas where our technical capabilities best contribute to the Defense Programs mission strategy. The Laboratory will help maintain the nation's tritium stockpile by supporting DOE's plans to produce tritium for the weapons stockpile in commercial light water reactors. This technology is based on designs and fabrication processes developed at our Laboratory. The Laboratory will also provide support with safeguarding and securing the nation's nuclear materials. Specific R&D areas include:

- development of a reactor-specific design of the tritium-producing burnable absorber rods (TPBARS) for the first tritium production mission
- transferring technologies needed to design and fabricate TPBARS to the commercial sector



Since the Laboratory's inception in 1964, scientists and engineers at the Pacific Northwest National Laboratory have been advancing nuclear science and technology across the nation and around the globe.

- demonstrating tritium extraction processes to provide design bases for the Tritium Extraction Facility
- evaluation of methods and materials for improving the effectiveness and reducing the costs of TPBAR components.

Other areas in which Pacific Northwest National Laboratory will support the weapons thrust area include:

- assisting Defense Programs in interpreting safeguards and security policies and identifying cost-effective implementation procedures
- consulting to the DOE weapons laboratories
- providing technical expertise to support DOE environmental compliance on defense missions
- supporting DOE in the safe disposal of excess weapons-grade plutonium.

4.4.3.3 Office of Counterintelligence (DOE-CN)

Pacific Northwest National Laboratory supports the DOE Office of Counterintelligence by enhancing counterintelligence (CI) capabilities through the development of relevant technologies and the implementation of special processes that will assist in ongoing local and national efforts to protect the Laboratory and DOE National Nuclear Security Administration personnel, assets, classified sensitive programs, and sensitive information from adverse intelligence and terrorist activities of foreign entities and their agents. Three over-arching goals articulate the Laboratory's strategy to achieve this mission:

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

In accomplishing these goals, the CI program executes its responsibilities with recognition of the importance of preserving an open, but appropriate, scientific environment, to include sound management of foreign interactions beneficial to national security interests.

The Laboratory CI program is comprised of three separate elements assigned to the National Security Directorate. One element is the CI program organization with primary responsibility for the essential CI mission responsibilities defined in the Laboratory DOE contract. These responsibilities include: protect DOE/NNSA classified sensitive programs and information, personnel, and assets from foreign intelligence and international terrorists activities; and detect and deter trusted

insiders who would engage in activities on behalf of a foreign intelligence service or terrorist organization. The two other significant elements that comprise the Laboratory CI program include special teams that support DOE-CN projects involving its Information/Special Technology Program, in particular the Inquiry Management and Analysis Capability coupled with its Operational Analysis Center, the CN Inspection Program, and the DOE Polygraph Program.

The Laboratory CI program continues to be extremely effective in executing its mission responsibilities and has grown into one of DOE's largest and most active CI efforts. PNNL has fully integrated key elements of DOE-CN's 2002 strategic plan into all aspects of CI project management and the integrity and reputation of the scientific community is enhanced to a degree that positively impacts the Laboratory's potential to achieve its defined mission.

4.4.3.4 Office of Intelligence (DOE-IN)

Pacific Northwest National Laboratory continues to be a leading provider of technical analytical support to the DOE Office of Intelligence. We perform technical analysis and computational modeling that addresses national issues in nuclear weapons materials production, nuclear and non-nuclear energy resources, environmental security, information operations/information warfare and cyber security and other tasks as appropriate. As part of our DOE Work for Others program, we perform a wide range of related analytical work for other government intelligence community organizations, including major commands within the Department of Defense.

4.4.3.5 Office of Security (DOE-SO)

Pacific Northwest National Laboratory supports the DOE Office of Security and Office of Emergency Operations through program leadership and development and application of technologies and tools that provide for the protection of our nation's most critical physical resources and infrastructure. Although the common theme is counterterrorism, our collective work has a broader focus with key contributions in developing technologies, processes, and capabilities that help promote the security of our homeland against internal and external threats.

Safeguards and Security

Pacific Northwest National Laboratory is involved with protecting special nuclear materials and government property across the DOE complex. In conjunction with the Washington Group International, Inc., and the DOE Chicago Field Office, we ensure that appropriate safeguards and security interests are protected and controlled at the Pit Disassembly and Conversion Facility, which will be located at the Savannah River Site. At the Hanford Site, the Laboratory supports the Hanford Safeguards and Security Program. Under the auspices of the DOE Office of Security, the Laboratory and the Army Special Forces perform vulnerability assessments and conduct force-on-force security exercises at various DOE sites.

Information Security and Critical Infrastructure Protection. In the areas of information security and critical infrastructure protection, the Laboratory has developed information visualization technologies (Starlight and Spire) that present a visual representation of text and other data in formats that are natural for the human mind to assess. Both are being used to analyze network transcripts and

Pacific Northwest National Laboratory's science-based capabilities for national security applications are significantly enhanced through our Laboratory Directed Research and Development program.

connection logs to help identify actual and potential cyber intrusions at over 100 defense computer sites around the world. A similar program supports DOE needs.

Information Security Resource Center. The Information Security Resource Center provides technical assistance for DOE's security programs, requirements, and countermeasures. The Information Security Resource Center is networked into the resources of the national laboratories and other federal and industrial organizations to promote, develop, and provide training, and support information assurance initiatives. The Center supports initiatives in information security, power grids, and the national information infrastructure to keep pace with related technology innovations and evolving cyber threats to the nation's critical infrastructures. Technology developments like Secure Safe and the development of the electronic OPSEC Internet Assessment Guide (MOZART) are providing new ideas and concepts to current programmatic issues. The Incident Tracking and Analysis Center is providing policy development, tracking and trending capabilities, and analyzing the information on the Incidents of Security Concern Program to assist in training development and requirement identification.

Information Assurance Outreach Program. The DOE Office of Security established an information assurance outreach program to provide the nation's energy industries with access to skills and expertise developed for the protection of information assets. This effort is consistent with the findings and recommendations of the President's Commission on Critical Infrastructure Protection and assists DOE with the discharge of its responsibilities mandated by Presidential Decision Directive 63.

Cyber Security R&D

The Pacific Northwest National Laboratory Cyber Security R&D Program includes the Critical Infrastructure Protection & Analysis Laboratory, which developed from a Laboratory initiative, a dedicated Cyber Security Research Team, and a suite of over 20 ongoing research projects specific to cyber security and information assurance. Its research agenda ranges from insider threat technology, to advance security analytical methods, to component-based security. The program collaborates with universities and industry to leverage the best resources available to address cyber security issues of national concern. A broad range of government institutions and industry sponsor the wide range of ongoing cyber security R&D.

Critical Infrastructure Protection and Analysis Laboratory (CIPAL)

Pacific Northwest National Laboratory dedicates the Critical Infrastructure Protection & Analysis Laboratory to cyber security R&D including Information Assurance, Information Exploitation, Information Operations, Computer Network Defense, and Computer Network Exploitation. CIPAL includes an extensive isolated heterogeneous network (computers, switches, routers) with capabilities to synthetically generate Internet traffic real-time in many forms effectively simulating the Internet. Its TrafficBot generates normal Internet traffic while its Coordinated Attack Tool can superimpose exploits creating a rich environment for cyber security research, and the performance testing of new concepts, technologies and tools. The CIPAL assets can also be used on performance and stress test existing COTS/GOTS/public domain security products under consideration for deployment. CIPAL is accessible to others for cyber security R&D and performance testing.

Transportation Security. Over the past several years, Pacific Northwest National Laboratory has pioneered the development of microwave and millimeter-wave holographic surveillance systems for transportation security. This development responded to a need by the Federal Aviation Administration, airports, commercial airlines, and the traveling public for a personnel surveillance system capable of detecting concealed weapons fabricated from plastic and ceramic and explosives made out of liquid and plastic.

4.4.3.6 Counterterrorism and Homeland Security

Pacific Northwest National Laboratory supports a number of clients with national security missions in the areas of countering drug smuggling, combating terrorism, crises and consequence management, law enforcement, and forensics. These clients include: Office of National Drug Control Policy; Office of Homeland Security; Department of Treasury; U.S. Customs Service; Internal Revenue Service; Bureau of Alcohol, Tobacco and Firearms; Department of Justice; Federal Bureau of Investigation; Immigration and Naturalization Service; and Federal Emergency Management Agency.

Examples of our work supporting counterterrorism and homeland security for these clients include basic and applied research and development of new statistical forensic techniques to assist law enforcement in the identification, collection, and preservation of trace evidence. We also developed the Acoustic Inspection Device, a technology product designed for acoustic inspection of sealed containers, and the Millimeter Wave Holographic Imaging System that will inspect and detect contraband and weapons carried in crowded and sensitive areas. Research and development has been pursued on supercritical fluid extraction, Raman laser spectroscopy, matrix assisted laser desorption, and ion mass spectrometry.

We have developed sensors to interdict radiological and nuclear threats as they cross international borders, and have trained and equipped domestic and international border guards and inspectors to interdict weapons of mass destruction using these advanced sensors.

Training programs also have been developed for international first responders (police, fire, medical) to help them evaluate, assess, characterize, and manage the emergency response to an act of terrorism involving weapons of mass destruction.

A significant aspect of our national/international homeland security programs is the close linkage to and leverage of other Hanford resources such as the Hazardous Materials Management and Emergency Response (HAMMER) training center.



While the terrorist attacks of September 2001 heightened society's focus on research and development activities in support of national security and counterterrorism, Pacific Northwest National Laboratory has been working in this area for decades. Many of the Laboratory's scientists and engineers have devoted their lives to conducting research and developing technologies that help keep America – and the world – safe.

4.4.4 Capability Development: Role of Laboratory Initiatives

While we cannot predict the future evolution of the U.S. national security strategy, our ability to support DOE's national security mission depends on continuously renewing our internal capabilities, in terms of people, facilities, and equipment. Laboratory Directed Research and Development initiatives at both the Laboratory level and within the research directorates support the DOE research and development portfolio objectives in a multitude of ways and the synergy between mission focus and capability development increases as each research and development project is completed and the relevant technologies transition and grow into other application areas.

This document addresses the Laboratory-level Laboratory Directed Research and Development initiatives in greater detail in the Major Laboratory Initiatives section of this plan. However, summaries of the current National Security sponsored initiatives are provided below to amplify the important linkage of these Laboratory Directed Research and Development programs to the overall National Security and DOE missions.

The **Infrared Sensing initiative** is expanding the Laboratory's role in developing infrared sensors to detect and identify chemical effluents in the environment. This research supports all of the DOE national security mission requirements that are reliant on remote effluent detection and characterization. Other national security needs include battlefield NBC defense, intelligence collection and targeting, battle and collateral damage assessment, and communication. Civil applications include atmospheric science, weather prediction, transportation issues, and industrial and agricultural process control. Federal funding for national security infrared applications has grown 40-fold in less than 10 years to a projected volume exceeding \$500 million in fiscal year 2002, and DOE roles and requirements are expanding. Within the Laboratory, infrared-related programmatic research is expanding rapidly. Recent development of infrared chemical sensing techniques based on frequency modulated spectroscopy and quantum cascade lasers at Pacific Northwest National Laboratory has the potential to render conventional approaches to chemical detection obsolete.

The infrared sensing initiative was completed at the end of fiscal year 2002. Because of the initiative, the Laboratory's breadth and depth of technical capability in critical components of infrared sensing are considered unique among the DOE laboratories.

The **Imaging Science and Technology initiative** is developing new image processing algorithms, image fusion methodologies, and three-dimensional visualization tools for multiple domain applications to meet the challenges related to the generation and interpretation of large, multidimensional images at various scales in many fields. Specific focus includes 1) remote sensing of the earth for national security and natural resource management missions, 2) cell imaging for scientific investigations of systems biology, and 3) ultrasonic imaging of engineered materials for energy applications. Ultimately, the goal of the initiative is to enable end-users to gain greater value and insight from image-based investigations, to improve the productivity and accuracy of image analysis, and to bring about more effective data interpretations and decision outcomes.

The **Advanced Nuclear Science and Technology initiative** provides an integrated science program in actinide science; radiation materials science; computational modeling; and advanced diagnostics, prognostics, and controls. The initiative builds on our existing capabilities and expertise to establish the Laboratory as a leader in selected nuclear science and technology focus areas. The initiative provides a focused mission framework and vision for programs, staff, and facilities that will advance nuclear science and technology to meet the needs of the Department of Energy and DOE-linked U.S. government agencies and strategic objectives in the 21st century. The initiative will consider nuclear science for national security, environmental management, basic science, medical uses, and both current and future nuclear power applications areas. Fiscal year 2003 will be the second full year for the Advanced Nuclear Science and Technology initiative.

Our new **Homeland Security Initiative** (new start in fiscal year 2003) is focusing on making investments that will significantly advance the flexibility and effectiveness of technologies for anticipating, preventing, and responding to a broad base of threats against our people and assets. The initiative focuses on the use of advanced materials and sensors for improved collection, separation, and detection of threat agents, and on the development of new analytical, statistical, and computational methods to manage the enormous and diverse sets of information related to recognizing and communicating threats. Our long-term strategy also includes leadership in evaluating the efficacy and implementation trade-offs of proposed detection and information technologies, including the creation of a technology testing and evaluation capability.

In addition to the focused benefit of the Infrared Sensing, Imaging Science and Technology, Advanced Nuclear Science and Technology, and Homeland Security initiatives, we also find significant contribution to national security mission needs coming from other Laboratory Directed Research and Development efforts as well.

- The Computational Sciences and Engineering initiative is developing advanced methods of analyzing data applicable to interpreting satellite information, forensics tools, and critical infrastructure protection.
- The Nanoscience and Nanotechnology initiative is developing capabilities that will result in a new generation of enhanced sensors and sensor arrays, light emitting devices (lasers and diodes), nanoscale separations technology over a macroscopic area, fuel production, photo detection and photo catalyst systems, and the modeling and simulation capabilities needed to understand and fully exploit the chemical and physical properties operative at this scale.
- The science resulting from the systems biology investments will play a critical role in understanding and countering the effects of biological warfare agents on the human body, food, and water supplies, and for identifying and characterizing biological agents of mass destruction.

Our work supporting counterterrorism and homeland security includes basic and applied research and development of new and novel forensic techniques.

Operations and Infrastructure Strategic Plan

5.1 Enabling Science and Technology Excellence Through Best in Class Laboratory Management, Stewardship, and Operations

To deliver breakthrough scientific discoveries and then rapidly translate them into applications for our customers, we must achieve and sustain new levels of leadership and outstanding performance in managing this research enterprise.

To be best in class we are pushing the boundaries for excellence in all areas of Laboratory management and stewardship.

This vision extends to our commitment to

- produce **outstanding managers and staff** who are at the highest levels of engagement, productivity, and excellence in their disciplines, and who recognize the Laboratory for the opportunities offered by its premier research work environment
- achieve **benchmark standards for laboratory management and operations** in which our facilities and equipment, work practices, operational environment, and management systems represent the new standard of excellence among national laboratories
- establish the Laboratory as **an integral and highly valued part of the region's science and technology network through** our contributions in solving the region's significant technical challenges, supporting economic development, advancing science education, and improving the quality of life.

Our staff, our facilities and equipment, our management systems, and our operational environment must perform at the highest levels of productivity and operational efficiency if we are to enable the Laboratory to reach its full potential. In pursuit of this vision, we will be recognized as the benchmark for laboratory management and operations as measured against other national laboratories and similar institutions.

This means that we are the most effective and efficient laboratory at delivering excellent research, maintaining outstanding operational practices, and providing long-term stewardship. We are committed to excellence in laboratory operations and management and will make continuous improvement investment in three areas:

Laboratory Competitiveness

- We develop a highly engaged workforce led by talented managers who are recognized as best in class.



Pacific Northwest National Laboratory supports its vision to be best in class in part through its contributions in advancing science education.

- We will maximize science and technology productivity for the lowest possible cost using our balanced portfolio approach for cost efficiency management.

Enabling Research

- Our management systems anticipate and respond to changing program needs, enable interdisciplinary teaming, and promote graded management of technical and operational risk.
- Our safety, security, and environmental responsibilities are fully embedded in how we conduct our daily work and assured through our self-assessment program.

We substantially increase our scientific productivity through improved work practices.

Laboratory Stewardship

- We are committed to the long-term stewardship of the Laboratory.
- We develop and maintain forefront research facilities and equipment, which enable program growth, innovation, and broad collaboration.

The first part of this section describes the Laboratory's approach to performance-based management, which is a critical enabling mechanism for assuring Laboratory management and DOE that we are achieving the expected performance outcomes. This section also addresses areas that the Laboratory will pursue to further strengthen particular elements of performance-based management.

The remaining sections provide greater detail on core elements of how we will bring the best private-sector laboratory operations practices to support the management of the research programs and facilities. These functions cover the following areas:

- Human Capital—providing expertise and guidance for selecting and developing leadership that inspires our workforce and attracts the new talent needed to sustain and achieve critical mission outcomes.
- Environment, Safety, and Health Management—facilitating the creation of a safe, fully compliant work environment in support of mission outcomes.
- Safeguards, Security, and Nonproliferation—serving to protect the Laboratory's physical and information assets, including classified matter, nuclear material control and accountability, and computer and network systems security.
- Information Resources—providing stewardship for updated and networked computer systems in support of Laboratory missions.
- Communications and Trust—ensuring the Laboratory's commitment to be a valued and trusted community and regional asset.

Achieving and sustaining operational excellence requires a sound and systematic approach to performance-based management throughout the Laboratory, supported by an effective partnership between the Office of Science, the Richland Operations Office, and Laboratory management. This partnership remains a key component in supporting the Laboratory's ability to focus on the most critical mission, stewardship, and operational outcomes.

5.2 Performance-based Management

Pacific Northwest National Laboratory is committed to achieving the highest standards of scientific and operational excellence for the Department of Energy and all of our stakeholders. As we pursue these outcomes, an enhancement in management philosophy is taking shape that will guide the Laboratory for the next several years. Using a joint model of laboratory governance, DOE and Laboratory management are creating a set of contractual relationships where the stewardship of DOE assets is ensured by the use of best industry practices and systems. Through this new contract, the Laboratory will provide enhanced assurance of system adequacy, operational performance, and cost effectiveness by using a combination of self-assessment, internal oversight, external regulatory oversight, and independent third-party certifications.

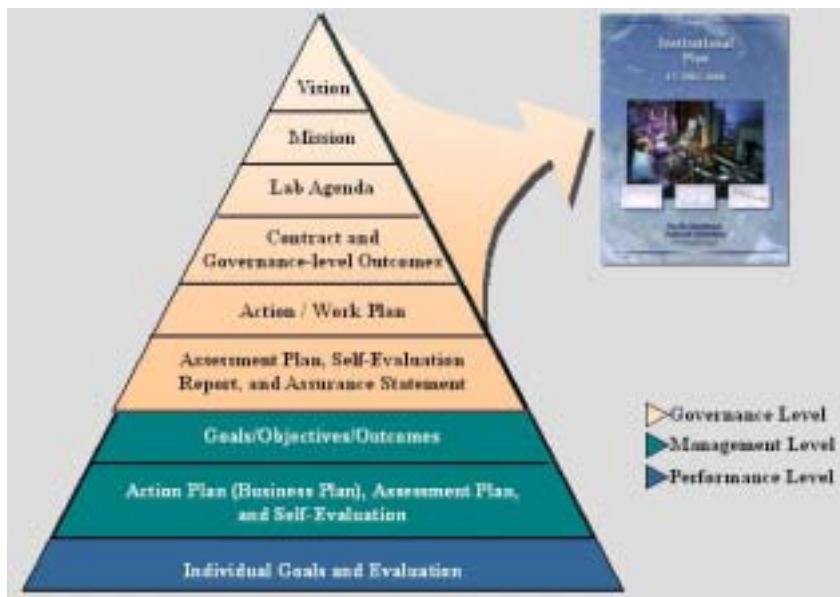
To support these levels of performance excellence, our strategy is to use a best-in-class performance-based management system. Performance-based management forms the core approach for Laboratory management to align and integrate strategy, processes, people, technology, and knowledge in order to ensure that the Laboratory produces results that are valued by our customers and stakeholders. Key to the success of performance-based management is that managers and staff are committed to delivering science and technology excellence for our customers, continuing to improve overall organizational and operational effectiveness, and building an environment of organizational and personal learning.

An effective performance-based management system begins with a clearly defined accountability framework for leaders and managers. Key management processes allow for communication of goals and strategies within the accountability framework. The function of Laboratory senior management is to partner with the DOE to set the vision, goals, and strategies for the Laboratory; approve the acceptable levels of risk; allocate resources; and monitor and maintain an integrated view of overall Laboratory performance against strategic goals and objectives. The function of management is to deploy the resources approved by senior leadership, monitor performance to accomplish research objectives, and deliver the necessary performance information to senior managers to support their efforts in monitoring and integrating performance across the Laboratory. The role of staff is to perform work while meeting the performance expectations set by management. The model uses internal review and assurance functions to provide oversight and feedback on the effectiveness of controls to achieve our goals.

Performance-based management is supported by many processes throughout the Laboratory but the foundation is a strong self-assessment process used by line



Performance-based management assures value by focusing the organization on our customer's desired outcomes.



The Institutional Plan is the starting point for our performance-based measurement system. Goals and objectives of the Laboratory are communicated through the organization to individuals performing the functions of our laboratory operations.

management. Leaders and managers at all levels are accountable to gather and regularly monitor performance information by using the tools and processes of self-assessment to ensure that

- optimal (acceptable/unacceptable) levels of risk and performance expectations are determined during the planning process as the basis for decision-making involving resource allocation and prioritization
- resources are continually monitored and aligned to achieve success against planned strategic and operational outcomes
- operational and other performance issues that need attention are identified and elevated to appropriate levels for management evaluation and continuous improvement actions

- performance feedback and results are communicated and used to strengthen and improve business results, promote organizational learning, and enhance strategic decision-making.

Performance-based management has been used by the Laboratory for a number of years and has become an integral part of the way we do business and the results we are achieving. We believe, however, that there are opportunities for improving the value and effectiveness of performance-based management, particularly in terms of line management’s ability to integrate our planning and assessment process. In particular, performance information and analysis improvements will optimize decision-making, better prioritize and deploy our resources, and achieve greater cost effectiveness. The following sections provide additional discussion on the Laboratory’s plans for strengthening performance-based management.

5.2.1 Integrated Planning and Assessment

From the time that the Laboratory first began implementing performance-based management in 1996, planning and systematic measurement of performance against plans have been our principal management tools for achieving Laboratory strategic goals. In fiscal year 2002, the integrated planning and assessment systems were combined into a single management system. This system’s tools help Laboratory management improve the overall alignment of Laboratory strategies and goals with the DOE strategic objectives and to create better internal organizational alignment. As a result, the Laboratory’s annual business planning process now includes the development of performance measures with updates to self-assessment plans as the mechanism that line managers use to regularly monitor performance against their business goals and objectives.

At year-end, managers analyze their overall performance results to assess strengths, determine improvement opportunities, and use the information as input to planning for the following year. This process results in the identification and prioritization of operational and financial risk areas that are reviewed by the Leadership Team and incorporated into plans to support Laboratory strategic objectives. Laboratory senior management also oversees Laboratory-level processes that are used to define performance issues and improvement areas, based on their potential impact to Laboratory strategic goals and objectives.

The Operations Improvement Initiatives support the goal of providing staff with useful, cost-effective, and hassle-free work processes. Through the Operations Improvement Initiatives, any Laboratory-level or management system has the opportunity to submit a proposal to request funding for special upgrades, equipment, tools, etc., for improving laboratory services and support during the annual planning and budget setting process. These processes represent important and well-established elements of the Laboratory's approach to performance-based management.

Over the past several years, we believe that the strength of the Laboratory's planning and assessment processes has contributed significantly to the Laboratory's achievement of "outstanding" evaluations from the Department of Energy. We fully expect that the continued focus on better integration of planning and assessment will help drive increased value, added efficiencies and cost effectiveness for our customers, as well as further support our ability to reinvest targeted resources in the Laboratory's programmatic and scientific area. The following sections provide discussion and examples of additional results the Laboratory is achieving with its approach to performance-based management.

5.2.2 Management Systems and Continuous Improvement

To be recognized as the benchmark for laboratory management and operations, the Laboratory's management systems must be able to anticipate and respond to changing program needs, enable interdisciplinary teaming, and promote graded management of technical and operational risk. The first phase of development and implementation of management systems began in 1996 and continued through 2000. During this period, the Laboratory's approach was to ensure compliance with external regulatory requirements, improve operational performance, and continuously improve services and processes.

In fiscal year 2001, the Laboratory initiated an effort aimed at transforming our management systems to create more emphasis on facilitating the research and development process while ensuring compliance with requirements. Using a maturity evaluation process based directly on the Malcom Baldrige Award Criteria for Performance Excellence, each management system owner conducted an in-depth self-assessment to evaluate their overall effectiveness in supporting Laboratory needs and to identify improvement opportunities for individual management systems. Management system owners used the results from these evaluations to implement improvements that would benefit the work environment for research and development staff. Attaining the highest standards of excellence in science and operations requires the focused discipline of performance-based management and the constant pursuit of opportunities for improvement. As the Laboratory enters a period of change involving the shift toward use of best business practices,

our ability to access and use well-integrated performance information is vital to the Laboratory’s overall success. Our strategy-driven approach will support better integration of planning and assessment in order to help managers throughout the Laboratory make better business decisions, improve the way we prioritize and deploy resources, and implement methods for greater cost effectiveness.

For example, an important enhancement will be the incorporation of risk management principles into the planning process as the basis for decision-making involving resource allocation and prioritization. Processes will be established to enable operational and performance issues that need attention to be identified and elevated to the appropriate management level for evaluation and continuous improvement. We will also establish new methods for using the results from performance reviews and other feedback to enhance strategic decision-making and promote organizational learning. Continued maturity in performance-based management will ensure that Pacific Northwest National Laboratory fulfills its performance outcomes to the Department of Energy and the nation.

5.2.3 Cost Effectiveness

The results of Laboratory management’s dedication and commitment to performance-based management speak for themselves. The Laboratory has a proven record of continuous performance improvement as evidenced by the summary of annual ratings received from DOE’s Richland Operations Office from fiscal year 1994 through fiscal year 2001 (Figure 5.1).

The Laboratory’s achievement of four straight “outstanding” ratings from fiscal year 1998 through fiscal year 2001 reinforces the importance that management places on continuous performance improvement in everything we do. In addition to helping us sustain high levels of overall Laboratory performance, we rely on performance-based management to help us identify opportunities for improved efficiency and effectiveness in all aspects of operational performance. Our management system owners use performance data to regularly monitor the performance and overall health of their management systems. By using perform-

ance information in this way, management system owners can more closely track the efficiency and effectiveness of their processes and use the results to support achievement of Laboratory-level cost management goals. This approach has helped the Laboratory maintain its overhead costs at stable levels. Pacific Northwest National Laboratory will continue to address cost reductions through focused review of costs, indirect resource expenditures consistent with strategic objectives, continual pursuit of cost reduction or avoidance opportunities, and documentation of benchmarks and baselines for results-based management. The focus on overhead cost reduction, however, will not be allowed to detract from the world-class science and technology being developed

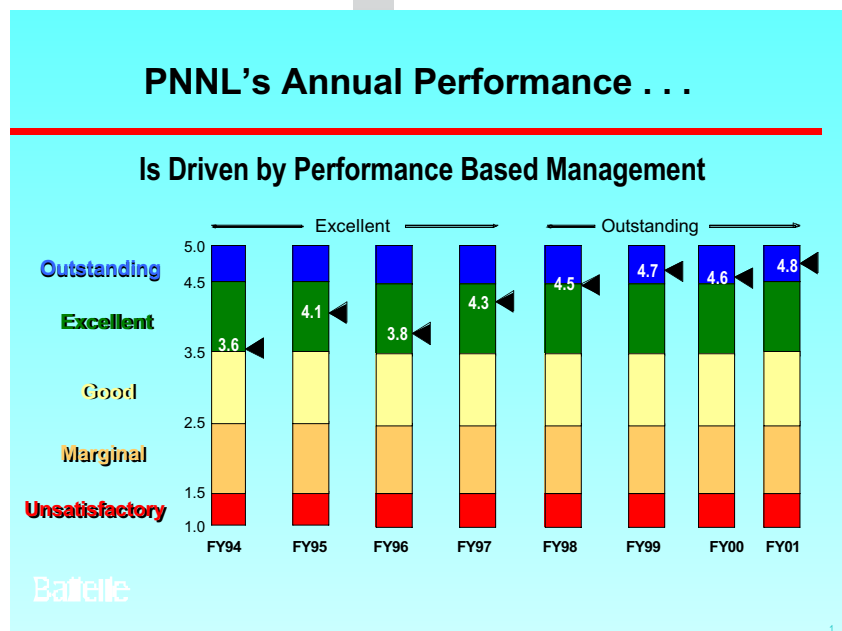


Figure 5.1. Performance Rating 1994-2001

at the Laboratory. The remaining sections provide further discussion of how Laboratory operations are achieving high levels of performance while supporting the Laboratory’s goals of efficiency and effectiveness.

5.3 Human Capital

Pacific Northwest National Laboratory’s human capital strategy is designed to provide the Laboratory with extraordinary leaders and talented staff who create an exhilarating work environment that achieves excellence in all facets of Laboratory stewardship. This stewardship includes distinction in science, technology, laboratory operations, community relations, and workforce diversity. An innovative climate of excellence with an emphasis on individual achievement and team collaboration is the desired outcome.

Critical to our success during the next decade will be our ability to identify and leverage core leadership and staff competencies toward the delivery of high-value science, technology, and innovation in support of the Laboratory’s strategic agenda.

The human capital strategy consists of the following core elements:

- enhancing the selection of leaders and staff through increased use of diagnostic technologies that effectively identify, and thus maximize, scientific leadership and intuitive talents and instincts
- retaining and growing a diverse workforce that optimizes staff discovery by providing for both individual achievement and organizational excellence through improvements in the quality of work life
- accelerating workforce planning in support of aggressive succession planning, hiring, and development of strategic staff capabilities, thus facilitating the optimal fit between human and job requirements
- understanding that great managers enable great staff, and that a mutually reinforcing work climate is achieved when the energies of talented research teams are directed toward complex problems
- collaborating with division management through a distributed human resource management network, thus promoting integration between scientific missions and outcomes and an engaged human resources workforce.

Achievement of this strategy is dependent on securing and retaining quality staff that find personal and professional fulfillment in the work

Table 5.1. Laboratory Staff Composition^(a)

Full and Part-Time Employees	Total #	(%)	PhD	MS/MA	BS/BA	Other
Managers	563	(15.0)	129	203	176	55
Scientists	982	(26.1)	489	258	223	12
Engineers	409	(10.9)	66	165	170	8
Management and Administrative	875	(23.2)	15	127	391	342
Technicians	208	(5.5)	0	3	14	191
Clerical	504	(13.4)	0	0	42	462
Craftsmen/Laborers	177	(4.7)	0	0	6	171
Service Workers	47	(1.2)	0	1	0	46
Total	3,765		699	757	1,022	1,287

(a) Data as of April 2002.

that they perform. To ensure that staff reach their potential and thrive in a work environment that supports innovation, Pacific Northwest National Laboratory is committed to continually enhancing staff capability, diversity, and the work environment.

In order to improve our ability to recruit more experienced mid-level career and senior scientific staff, we will continue to pursue with our regional universities and other academic partners the establishment of joint appointments that go beyond adjunct faculty status. In addition, we will develop resources to support a significantly increased number of sabbatical appointments for accomplished scientists from top research universities and laboratories.

Pacific Northwest National Laboratory’s implementation of this strategy is illustrated in its fiscal year 2001-2002 effort to understand and measure the motivational factors of scientific engagement across the Laboratory. A baseline of leadership and staff engagement scores are being set to allow measurement of progress toward national norms of excellence. In addition to this leadership emphasis, Pacific Northwest National Laboratory’s management skills development program has been expanded to strengthen succession candidate interpersonal skills required for exceptional research and development leadership.

5.3.1 Human Capital Demographics

As illustrated by Tables 5.1 and 5.2, Pacific Northwest National Laboratory’s workforce is composed of a diverse and talented cadre of staff with a breadth of educational background(s) and formal preparation.

Table 5.2. Equal Employment Opportunity^(a,b)

Occupational Codes	Staff		Minority		White		Black		Hispanic		Native Americans		Asian/Pacific Islanders	
	M	F	M	F	M	F	M	F	M	F	M	F	M	F
Manager	447 (79.4)	116 (20.6)	25 (4.4)	8 (1.4)	422 (75.0)	108 (19.2)	2 (0.4)	1 (0.2)	14 (2.5)	4 (0.7)	3 (0.5)	1 (0.2)	6 (1.1)	2 (0.4)
Professional														
Scientists	756 (77.0)	226 (23.0)	97 (9.9)	33 (3.4)	659 (67.1)	193 (19.7)	8 (0.8)	3 (0.3)	12 (1.2)	4 (0.4)	5 (0.5)	2 (0.2)	72 (7.3)	24 (2.4)
Engineers	341 (83.4)	68 (16.6)	29 (7.1)	5 (1.2)	312 (76.3)	63 (15.4)	2 (0.5)	0 (0.0)	10 (2.4)	2 (0.5)	2 (0.5)	0 (0.0)	15 (3.7)	3 (0.7)
Management/ Admin	433 (49.5)	442 (50.5)	34 (3.9)	45 (5.1)	399 (45.6)	397 (45.4)	6 (0.7)	2 (0.2)	18 (2.1)	19 (2.2)	4 (0.5)	4 (0.5)	6 (0.7)	20 (2.3)
Technicians	121 (58.2)	87 (41.8)	14 (6.7)	9 (4.3)	107 (51.4)	78 (37.5)	2 (1.0)	2 (1.0)	6 (2.9)	3 (1.4)	1 (0.5)	1 (0.5)	5 (2.4)	3 (1.4)
Clerical	13 (2.6)	491 (97.4)	1 (0.2)	73 (14.5)	12 (2.4)	418 (82.9)	0 (0.0)	16 (3.2)	1 (0.2)	44 (8.7)	0 (0.0)	5 (1.0)	0 (0.0)	8 (1.6)
Craftsmen/ Laborers	164 (92.7)	13 (7.3)	17 (9.6)	3 (1.7)	147 (83.1)	10 (5.6)	4 (2.3)	0 (0.0)	11 (6.2)	3 (1.7)	1 (0.6)	0 (0.0)	1 (0.6)	0 (0.0)
Service Workers	22 (46.8)	25 (53.2)	1 (2.1)	1 (2.1)	21 (44.7)	24 (51.1)	1 (2.1)	0 (0.0)	0 (0.0)	1 (2.1)	0 (0.0)	0 (0.0)	0 (0.0)	0 (0.0)
Totals	2,297	1,468	218	177	2,079	1,291	25	24	72	80	16	13	105	60

(a) Data as of April 2002.
 (b) Numbers in parenthesis () are %.

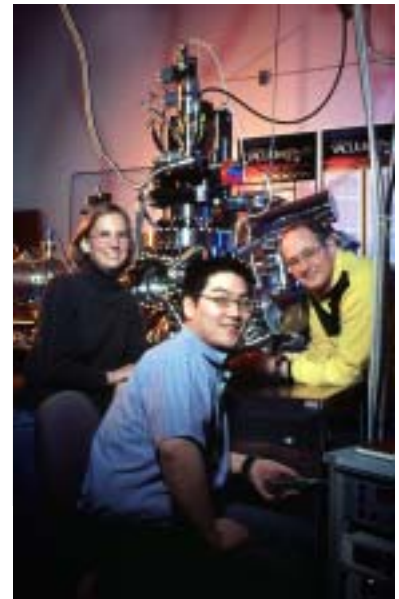
The career ladders within the Laboratory are being realigned during 2002 to clarify growth opportunities and to provide a more consistent pathway for staff to pursue their unique aspirations. Longevity of one's career is tied to a clear understanding of growth opportunities and contributes to a high retention rate of Pacific Northwest National Laboratory staff. The recent, 3-year average voluntary attrition rate is approximately 6% for staff losses. Exit interviews and other data are reviewed to understand and address the reasons that staff members leave, so that the Laboratory's work environment can be continually improved.

Pacific Northwest National Laboratory strives to be a good neighbor by supporting education, arts, and community projects. Our science education programs extend from elementary school students and teachers to postdoctoral students and university professors. We foster an early interest in science and math through classroom demonstrations. We encourage economic diversity and growth through a variety of programs to attract businesses to the area and support local business development and expansion.

Diversity Emphasis. Every level of management is responsible for advancing equal employment principles and applying genuine commitment to affirmative action in attracting and retaining a diversely talented workforce. Numerous programs are in place to increase awareness of employment opportunities for women and minorities. Strong relationships with local, regional, and national women and minority organizations are maintained to broaden career networks and contacts.

Noteworthy accomplishments in fiscal year 2002 include participation in a number of career fairs aimed at women and minorities including:

- National Organization of Black Chemists and Chemical Engineers
- National Society of Black Engineers
- American Indian Science and Engineering Society
- Annual Joint Statistical Meeting and Career Fair
- Society of Women Engineers
- Idaho National Environmental and Engineering Laboratory (Career Fair)
- Black Engineer of the Year Awards Conference and Career Fair
- Howard University
- University of Washington Fisheries Sciences Career Fair
- Texas A&M
- New Mexico State University
- Heritage College
- Washington State University
- University of Idaho
- Columbia Basin College



The Pacific Northwest National Laboratory attracts and retains diverse, talented employees who work together in interdisciplinary teams to solve today's pressing problems.

Staff involvement in community outreach and collaboration projects is aimed at increasing Pacific Northwest National Laboratory's presence and support in this important area. Examples of these efforts include:

- The Vista Hermosa project—a local educational speaking series available to Hispanic community attendees
- Sponsorship of diverse Pacific Northwest National Laboratory participants at regional events—e.g., addressing the Professional Engineer Society Speakers banquet; leading a discussion on global warming at a local Native American college; presenting climate change issues to the Olympia League of Women Voters; addressing the Washington State's League of Women Voters on global warming and energy
- Sponsorship of the Mucho Dinero Hispanic Outreach event
- Sponsorship of the Fiesta de la Familia Outreach event
- Participation on the Hispanic Outreach Leadership Alliance board
- Participation and sponsorship in numerous community and regional events—e.g., inaugural Battelle Volunteer Fair; Seattle Northwest AIDS Walk; United Way Day of Caring; Wishing Star Bowl-a-thon; Reading For the Blind radio service; Chip in for the Cure Golf Tournament; Cancer Fund Raiser via the Tumbleweed Music Festival; Walk for Diabetes; and the community Concerts at the Pavilion.



Staff at the Pacific Northwest National Laboratory are involved in diverse community outreach projects such as Mucho Dinero, a Battelle-sponsored seminar about Hispanic business marketing.

Diversity programs at the Laboratory have continued to gain support and enthusiasm, creating an inclusive environment where individual differences are honored. Personal commitments from high-level managers, scientists, and engineers are made to identify and mentor women and minority staff members to gain the knowledge, experience, and exposure to qualify for promotions. Quarterly meetings with management are conducted to discuss progress on affirmative action goals and to identify areas needing focused efforts.

Diversity Recruiting. Aggressive recruiting efforts have resulted in percentage increases of women and minorities in several areas of employment, including representation among scientists and engineers and total Laboratory populations. The Recruiting Referral Program generated 13 female and/or

minority new hires during fiscal year 2001 and continues to add value during fiscal year 2002. The Scientist and Engineering Rotation Program provided technical job exposure, development, and transition assistance for diverse staff who recently joined the Laboratory's workforce. Mentoring has been an effective tool to advance and nurture staff as they are assimilated into Laboratory activities.

Competition for Talent. To appropriately compete for research and professional talent in a dynamic research and development market, the Laboratory must offer competitive salaries, cash rewards, recognition systems, and a flexible array of benefits aligned with today's worker in mind. A current partnership with the Department of Energy, Richland Operations Office has helped to invigorate our total compensation philosophy of competitive incentives and to accentuate variable pay alternatives whenever possible.

A joint effort is under way to establish the next 5-year contract for DOE that can be used as a pattern across the DOE laboratory network. Intense project development is occurring to streamline and create a structure that allows the Department to manage its stewardship of laboratory assets according to best industry practices patterned after commercial practices. Innovative, out-of-the-box strategies are sought to maximize value for both DOE and its contractor(s) through this grass roots collaboration.

While a foundation of competitive pay and benefits is essential to attract and retain talented staff, we believe that an enduring strategy requires a careful combination of intrinsic accouterments that appeal to the needs of scientific staff for quality research facilities and equipment, career growth, opportunity, challenge, and an inspiring and competent Leadership Team. The right mix of autonomy, purpose, achievement, and competitive compensation will distinguish the Pacific Northwest National Laboratory as the research employer of choice, well into the 21st century.

5.4 Environment, Safety, Health and Quality Management

The Environment, Safety, Health and Quality Directorate now integrates the supporting management systems that deliver environmental management, facility safety, radiological control, training and qualification, worker safety and health, quality, and Standards-Based Management System products and services to the Pacific Northwest National Laboratory. These management systems are designed to anticipate and respond to changing program needs, enable interdisciplinary teaming, and promote graded management of technical and operational risk. It is through these management systems that we embed the appropriate compliance measures into the Laboratory's processes and directly contribute to increasing scientific research productivity.

A portion of the Environment, Safety, Health and Quality Directorate is funded directly by the organizations that require their support services (research projects and overhead-funded activities). We strive to enable project and line organization managers to maximize control over their support costs and to safely, efficiently, and effectively accomplish their mission.

5.4.1 Overall Vision, Goals, and Objectives

We provide innovative services and systems that enable our research mission to be conducted in a safe, efficient, compliant, and environmentally sound manner. Our vision for Pacific Northwest National Laboratory is to be the benchmark standard for national research and development laboratories in the integration of environment, safety, health, and quality management into research operations. To achieve that standard of performance, our objectives are to

- establish a partnership business model that integrates conduct of research and management systems as a work process focused on supporting staff and managers in the execution of their work activities
- fully develop and deploy effective, innovative, and integrated management systems that anticipate and respond to changing work processes, deliver value-added tools, and promote a graded risk management approach to research

- more effectively enable science and technology by aligning our operational capabilities to support our research project needs, e.g., support personnel, facilities, and information technology tools
- be recognized for excellence in managing Pacific Northwest National Laboratory's environment, safety, health, and quality assurance resources
- maximize staff involvement in, and ownership and development of, environment, safety, health and quality policies, procedures, programs, and practices
- optimize customer satisfaction with our cost-effective services.

5.4.2 Current Laboratory Conditions and the Status of Integrated Safety Management

We have integrated environment, safety, and health requirements into our management systems as required by our operating contract with the Department of Energy.^(a) Major initiatives conducted since 1995 have established a firm operating basis for environment, safety, and health and conduct of operations. This capability was confirmed by the phase I and II validation of our Integrated Environment, Safety, and Health Program that we received from the Richland Operations Office in 1998.

Pacific Northwest National Laboratory is now focused on process maturity beyond the initial Integrated Safety Management validation. Following the 1998 Integrated Safety Management validation, the Laboratory embarked on a continuous improvement program to ensure that we sustain long-term operational excellence. The Laboratory has now obtained third party-verification, i.e., Department of Energy Voluntary Protection Program Gold Star recognition and ISO 14001 registration of its environmental management system.

- Our Integrated Environment, Safety, Health and Quality Management System sponsors and maintains the linkages with other supporting management systems to achieve the goals of the DOE's Integrated Safety Management, Voluntary Protection, and Environmental Management Programs. As part of continuous improvement, this management system also identifies, tracks, and addresses weaknesses in the integrated programs. Our highest priority improvement areas are radioactive material management, biological safety, and hazards assessment.
- In fiscal year 2001, we incorporated the Integrated Operations System as a formal element of our Integrated Safety Management. This enhances research operations by integrating hazard identification and communication, identification and tracking of training requirements, hazard mitigation through self-assessment, detailed work practices, and user access authorization and control. We will complete the deployment of the Integrated Operations System to all Laboratory facilities by the end of fiscal year 2003.
- The Pacific Northwest National Laboratory's worker safety and health program has been awarded Gold Star status in the Department of Energy's Voluntary Protection Program, established by DOE to recognize superior performance in worker health and safety. This program is a partnership among labor,

(a) DE-AC06-75RL01830 Modification M255, Clause I-64, entitled *Integration of Environment, Safety, and Health into Work Planning and Execution (June 1997)*.

management, and DOE to promote worker safety through employee involvement. It involves work-site analysis, hazard prevention and control, safety and health training, management commitment, and employee involvement.

- ISO 14001 registration was achieved in 2002 as planned. ISO 14001 is the internationally recognized standard of excellence in environmental management, and achieving registration is a clear way to firmly establish the “E” (environmental component) as an integral part of the Pacific Northwest National Laboratory’s Integrated Safety Management Program.
- In March 2002, the Quality and Standards-Based Management Systems were integrated into the Environment, Safety and Health Directorate. The Quality Management System provides Pacific Northwest National Laboratory staff with a standards-based Quality Assurance Program needed for the Laboratory to deliver high-quality products and services consistent with the needs, expectations, and resources of our customer base. The Quality Management System accomplishes this purpose through the generation of the Quality Assurance Program Description, partnering with other management systems in defining methods for implementation, and conducting internal assessments of program effectiveness. The Quality Management System provides Laboratory staff with three program descriptions (Calibration, Suspect and Counterfeit Items, and NQA-1), a Quality Engineering department-level business manual, and a Laboratory-wide process for quality problem resolution, all of which collectively support the implementation of the Quality Assurance Program. The Standards-Based Management System operates a policy and procedures system based on the most appropriate set of external requirements, management policy, and consensus standards applicable to the work conducted at Pacific Northwest National Laboratory. These requirements are translated into procedures and guidelines that are easily understood, simple to access, and readily implemented in a manner that enables the effective and efficient execution of research and development activities while appropriately controlling the risk associated with work. The procedures and guidelines are maintained accurate and current by active regulatory review and information integration, and relevant by involving those responsible for implementation.



5.4.3 Long-range Strategies to Maintain Effective and Efficient Integrated Environment, Safety, Health, and Quality Management

The following strategies are examples of our continuous improvement in Environment, Safety, Health, and Quality Management System activities.

We employ the Voluntary Protection Program approach to ensure employee involvement in our Integrated Environment, Safety, Health and Quality Management System. The Voluntary Protection Program Steering Committee submitted Pacific Northwest National Laboratory’s Department of Energy Voluntary Protection Program application in October 2000. The application was the first electronic application submitted on-line to a website interactive with live Laboratory systems such as the Standards-Based Management System, Integrated Operations System, and Assessment Tracking System. The Voluntary Protection Program at Pacific Northwest National Laboratory was formally reviewed by DOE in May 2001, with Gold Star status presented on July 25, 2001. Pacific Northwest National Laboratory

is the first Office of Science laboratory to receive the highest level of recognition within the Department of Energy's Voluntary Protection Program. Following ISO 14001 registration, the Laboratory will begin to explore the business case for using a third-party consensus standard such as Baldrige or ISO 9001 as a mechanism for enabling the continuous improvement of the Quality Program and more tightly integrating the Quality and Integrated Safety Management Systems.

The Hazard Analysis Initiative is a 3-year project designed to make improvements in the identification, evaluation, and mitigation of environment, safety, and health hazards. The project integrates and improves existing tools like the Electronic Prep and Risk, the Standards-Based Management System, and the Integrated Operations System to enhance the efficiency and effectiveness of research and development work planning and control. When complete, this tool can be expanded to address other issues relevant to research and development operations including security, quality, and property management. The project also anticipates the ability to deliver cost savings in terms of reduced labor for research and development work planning and fewer accidents and incidents.

The Training and Qualification Management System has avoided several million dollars in annual costs through the innovative use of web-based, computer-based, and alternative training delivery methods. A comparison of the Laboratory's training costs to similar industries using the benchmarking services of the American Society for Training and Development reveals that our training costs are less than half of industry averages although we train about 35 percent more staff. As our capabilities with web-based training have matured, so have our efficiencies. Although technology costs increase on an annual basis, we are now going into our fifth fiscal year of maintaining a stable average tuition per course.

The Radiological Control Management System implemented an operational improvement initiative to provide a new access control system. The objective of the project was to implement an easy to use application that can determine quickly and reliably if a worker has all the qualifications (internal dosimetry, external dosimetry, and training) listed on the applicable radiological work permit. This system provides a link between radiological access control and the Integrated Operations System. In addition, the application provides for the preparation and tracking of radiological work permits. This system is an innovative, efficient system that is in line with the PNNL 2010 vision of enabling research and protecting the worker. Additionally, the system will enhance transition to external standards and perhaps eventually to external regulations.

The Laboratory has an initiative to facilitate work with low-level radioactive tracers. The Radiological Control Management System is the lead on the implementation of a fiscal year 2002 operational improvement initiative to meet the Laboratory's long-term goal for efficient, innovative, cost-effective, and compliant systems that enable research while protecting the worker, the public, and the environment. The initiative includes development of a subject area that specifically addresses all aspects of work with low-level radioactive isotopes (volumetric release, dosimetry, posting, and movement of radioactive materials). The Department of Energy has



The ISO 14001 Certification obtained in November 2002, along with the validation of Integrated Safety Management in 1998 and the achievement of Voluntary Protection Program Gold Star Status in 2001, culminates the Triple Crown vision rolled out by the Leadership Team in March 2000. Pacific Northwest National Laboratory is the first Office of Science Laboratory to attain the Triple Crown in Environment, Safety and Health.

approved a volumetric release standard. The Radiological Control Management System will work with the Environmental Management Services Management System to complete these improvements.

A working group was formed in May 2001 to identify opportunities for improving the processes and procedures for managing radioactive material at Pacific Northwest National Laboratory. An operational improvement initiative was approved to address the judgments of need developed by the working group. The Facility Safety Management System is coordinating the operational improvement initiative with the Facility Operations and Maintenance Management System, the Environmental Management Services Management System, the Radiological Control Management System, the Safeguards and Security Management System, and line management. Completion of these activities will result in a more streamlined process that integrates across multiple management system requirements. It also will eliminate duplication of effort by staff trying to implement various management system requirements and will standardize the method that staff use for maintaining radioactive material inventories. This activity will result in an innovative, cost-effective process for enabling research while protecting the staff, the public, and the environment. Additionally, one outcome of this activity is determining the most cost-effective method for implementing a Laboratory-wide radioactive material inventory, which is critical for eventual external regulation.

The focus for the Standards-Based Management System over the next few years will be to enhance management system integration to better enable research and development work process effectiveness and efficiency. The aim is to increase management system integration where work processes (from the point of view of a research and development manager or staff member) cross multiple systems. The focus of the integration efforts will be on those processes that will have significant impact on critical research and development work processes.

5.4.4 Stewardship of Our Environment

Our Pollution Prevention Program's green lab approach to environmental stewardship incorporates environmental practices into the design, development, marketing, deployment, and use of Pacific Northwest National Laboratory's services and technologies. Our objective is to fully integrate pollution prevention into all Laboratory activities. Our goals are to reduce waste and support research.

The Pacific Northwest National Laboratory's use of ISO 14001 to evaluate and drive changes in the existing Integrated Environment, Safety, Health and Quality Management System will enable the Laboratory to: 1) embed pollution prevention in management systems and meet the requirements in Executive Order 13148; 2) rigorously evaluate other key components of the Environmental Management System (records management, corrective action management); and 3) establish environmental improvement goals and demonstrate continuous improvement.



Staff at the Pacific Northwest National Laboratory are stewards of the environment both on the job and in the community, by participation in events such as Earth Day.

Pacific Northwest National Laboratory's waste management organization is continuing to work with the research and development directorates and with Facilities and Operations staff to identify waste generation, management, and disposal options. Waste forecasting, planning, and costing tools will allow a more detailed costing of waste management activities, as well as life cycle cost estimates and waste minimization activities. We also employ options for treating waste on-site to reduce or eliminate future costs and liabilities.

5.4.5 Waste Management Activities at Pacific Northwest National Laboratory Funded by DOE

Variable waste chargeback was implemented in 2003. The fixed portion is funded by Pacific Northwest National Laboratory overhead, which supports our waste operations and management (current generation) activities by funding the fixed cost for activities (e.g., permitting, storage, assessment of subcontractor compliance and record keeping) needed to dispose of newly generated wastes. The variable waste management costs (e.g., disposal, transportation, packaging and materials) will be recovered directly from the generating project via a service center. The Office of Environmental Management funding previously obtained for Environmental Management Services is now being used for facility activities in the Radiochemical Processing Laboratory. This transition completes a three-year Laboratory-wide effort.



Waste management costs generated by activities in the Radiochemical Processing Laboratory are now recovered through the variable waste chargeback process.

5.4.5.1 Strategic Issues

Pacific Northwest National Laboratory's waste management organization is initiating a detailed review of its operational effectiveness and facility needs. The 300 Area accelerated clean up includes demolition of the 305-B facility which is a Resource Conservation and Recovery Act (RCRA) permitted Treatment Storage and Disposal facility. A determination will be made relative to future facility needs, RCRA permit requirements, and operational effectiveness relative to other waste disposal contractors.

5.4.5.2 Emerging Issues

The Department of Energy's new Radioactive Waste Management Order (435.1) was issued in fiscal year 1999. The Laboratory developed an implementation plan in coordination with the Hanford Site. The plan requires additional funding to incorporate new and revised requirements into its management systems and operating procedures. Funding for implementation of 435.1 will not be allotted from the Office of Environmental Management's budget for fiscal year 2003. Pacific Northwest National Laboratory is currently looking at funding alternatives and the possibility that only certain parts of 435.1 may be implemented.

Washington State has enacted an Ergonomics Rule, which must be implemented by 2003. This rule applies to Pacific Northwest National Laboratory because approximately 50 percent of Battelle's facilities are not on Department of Energy property and fall under the new Washington State Ergonomics Rule. When multiple standards or laws apply, Battelle's practice is to apply the most conservative standard or rule to the consolidated Laboratory. The actions needed to implement the requirement are being tracked via the Assessment Tracking System.

The Worker Safety and Health Management System developed actions as part of fiscal year 2003 business planning for improvement of the biological safety program at Pacific Northwest National Laboratory. These improvement actions are being tracked in the Assessment Tracking System and will result in improvements to effectiveness, innovation, and efficiency in enabling research while protecting the worker, the public, and the environment. Additionally, the improvements will position the Laboratory for achieving the PNNL 2010 vision, which includes more work scope requiring the use of biological agents.

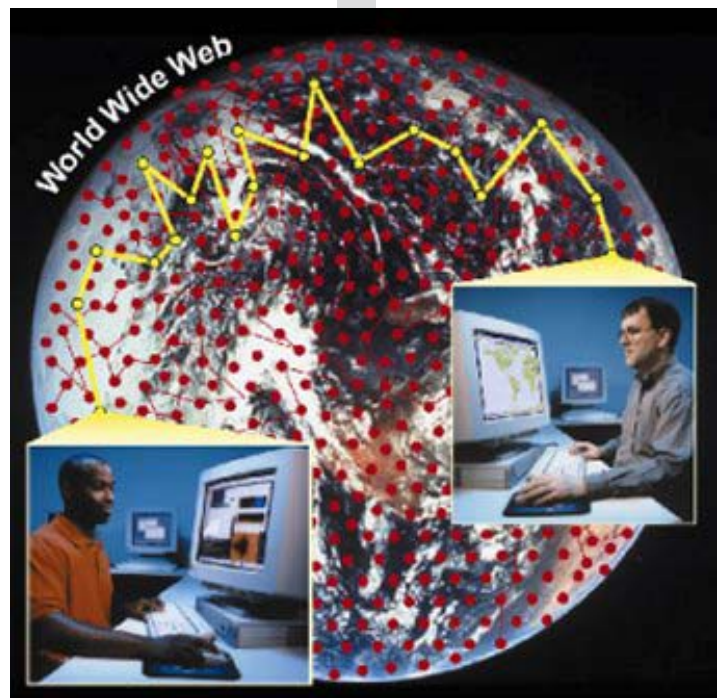
5.5 Security, Safeguards, and Nonproliferation

Pacific Northwest National Laboratory puts science and technology to work to solve problems for its primary customer, the Department of Energy, as well as for other government agencies and private industrial customers. In so doing, the Laboratory deploys an effective, ongoing safeguards and security program to support the Laboratory's research. This program enables research by facilitating an open and supportive research environment while ensuring appropriate levels of protection for information, assets and property, personnel, and nuclear materials. The Laboratory's safeguards and security program consists of the following standard broad areas:

- safeguards and security program management
- physical security and protection operations
- information security
- nuclear material control and accountability
- personnel security (including foreign visits and assignments)
- cyber security.

These program elements work together in conjunction with a counterintelligence program and an export control program to ensure appropriate protection and control of Laboratory assets while ensuring that the Laboratory remains appropriately accessible to visitors for technical collaboration.

Safeguards and security employs performance management practices integrating planning and assessments using a performance agenda, self-assessments, and improvement initiatives as deployment mechanisms. Performance is measured and monitored on a regular basis. Through self-assessment and reviews, safeguards and security is able to modify behaviors within the organization to achieve the strategic outcomes and mission objectives necessary for success. Identified performance metrics link directly to the vision and mission of the directorate as well as to the Laboratory and, through systematic data collection, provides information for use in making business decisions and determining improvement actions demonstrating the continual organizational learning process.



The Laboratory's Safeguards and Security Program covers many broad areas, including cyber security.

Safeguards and security's ability to execute an efficient management system and organizational structure that effectively maintains high operational standards, ensures customer satisfaction, and meets applicable compliance and regulatory standards is critical in the 21st century. Safeguards and security will continue to concentrate on improving management practices, increasing productivity and employ outcome-oriented performance measures to support operations contributing to the Laboratory's success and PNNL 2010 vision.

Pacific Northwest National Laboratory is a multiprogram Laboratory rated by DOE as a Class A facility. This designation denotes the relative importance of a facility in relationship to other DOE facilities and to the security and common defense of the United States. Class A facilities may engage in administrative activities considered essential to the direction and continuity of the overall DOE nuclear weapons program and are authorized to possess Top Secret matter or Category I quantities of special nuclear materials. The Laboratory does not possess Category I quantities of special nuclear materials but does possess lower category quantities of special nuclear materials and classified matter. As such, commitments for the protection of special nuclear materials and classified matter are priorities for the safeguards and security program. Protecting information, intellectual property, and physical property is a vital commitment in the Laboratory's institutional and operational philosophy.

5.5.1 Nonproliferation

Through the National Security Directorate, the Laboratory provides support to DOE's national security mission (including monitoring nuclear treaties and agreements, preventing and detecting proliferation, promoting international nuclear safety, countering weapons of mass destruction terrorism, and contributing to maintaining the U.S. nuclear deterrent). Accordingly, most requirements involving nonproliferation and counterintelligence have minimal direct impact on the Laboratory's research mission.

5.5.2 Integrated Safeguards and Security Management

In addition, an Integrated Safeguards and Security Management (ISSM) program has been developed and implemented, one of the first in the complex. This program integrates safeguards and security requirements into the processes of planning and conducting work at the Laboratory and assists management in addressing identified threats and associated risks. It ensures that all safeguards and security elements work together effectively to provide a strong, protective umbrella for long-term business strategies. Over the past few years, the ISSM program has undergone several assessments and implemented actions to promote the continued maturity of its deployment with a focus on performance-based security management. Actions developed and completed in response to these assessments included leveraging best practices and processes from the Integrated Safety Management program, and the integration into mainstream Laboratory processes such as the Standards Based Management System, Integrated Operations System, Electronic Prep and Risk System, and others continues to strengthen the ISSM program. Building a system that met the



protection needs for both the science and security environments was essential, and the Laboratory has evolved the maturity of the ISSM system to accommodate both effectively.

Recommendations from the Commission on Science and Security study are being addressed through our ISSM program. Roles for security responsibilities are being clarified to include reinforcement of the line organization's primary responsibility in this area. Line organizations participate in the decision making processes on all matters including security. Feedback from directorates is obtained and used by the security and safeguards program to improve and expand the program. An Integrated Safeguards and Security Senior Management Council has been established and chartered to provide a senior forum for the review of new and changing security and safeguards 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. The council is comprised of the Deputy Laboratory Director for Operations, the Director of Facilities and Operations, the Manager of Safeguards and Security Services, the Chief Information Officer, the Senior Counterintelligence Officer, the Computer Protection Program Manager, and a representative from the Environmental Technology, National Security, Energy, and Fundamental Sciences research directorates. This representative group makes sure that all equity stockholders are represented in addressing and implementing safeguards and security related issues.

A broad risk-based approach for security management practices is also a primary initiative. The Laboratory employs a system-wide approach for assessing risks associated with assets and comprehensively determining priorities for the protection of those assets. In this way, resources may be balanced in accordance with the risk for a more economical and effective protection strategy. Asset Protection Agreements have been developed and implemented to document this approach.

5.5.3 Information and Asset Protection

We are aware that threats to scientific and technological information and programs continue to exist. The Laboratory has a very proactive safeguards and security program to ensure that appropriate measures are employed to discourage or defeat attempts to collect information or disrupt operations. Defense against loss, theft, sabotage, and espionage is an essential consideration for DOE program activities, cooperative research and development activities, and work for others, and is consistent with the following current and long-term safeguards and security program priorities:

- physical protection, control, and accountability for nuclear and special nuclear materials
- protection of classified matter
- protection of physical and intellectual property (which includes operating facilities, sensitive information, sensitive property, and equipment)
- assurance that the safeguards and security performance objectives and supporting milestones agreed upon by Pacific Northwest National Laboratory and DOE are conducted in a cost-effective manner.



Pacific Northwest National Laboratory applies the latest security technologies to protect its valuable information assets.

Many elements of the standard safeguards and security program contribute to the effective protection of information at the Laboratory while ensuring appropriate support of research.

The Laboratory employs a graded system for the protection of property, facilities, information and assets that includes the use of security areas, access controls and accountability systems. Asset Protection Agreements (APAs) are developed to document the identification of the security interest activities and associated protection measures by facility location. APAs are established on a graded fashion and take into account the nature of the security interest, protection requirements identified

in appropriate directives, threat potentials, and countermeasures, and assign a defense or safeguards priority position based on a composite evaluation of these factors. The APA serves as the security plan for the individual facilities. Line management assisted by Safeguards and Security Services determines the protection plans. The APA is an automated system that receives input directly from other applicable Laboratory systems involving different security interests/assets on a near real-time basis. This information is then reviewed to ensure appropriate security measures have been put into place.

Safeguards and security is also represented on the Laboratory's Institutional Biological Safety Committee. Security guidance is provided to the committee to assist in the decision-making processes (approval/disapproval) for current and future bio-safety work activities at the Laboratory. This representation is additionally directly involved in the planning processes for the proposed bio-safety Level 3 Laboratory activities to ensure adequate security is afforded without impacting research.

5.5.4 Information Security

Information security measures address the protection and control of classified and sensitive information. Information security also ensures that individuals effectively protect the information to which they have access or custody. The information security program includes

- operations security
- classified matter protection and control, including security of foreign intelligence information, sensitive compartmented information, and special access programs
- communications security and technical surveillance countermeasures
- protection of unclassified controlled nuclear information, official use only information, naval nuclear propulsion information, and other sensitive information.

The information security program establishes a protection and control system that requires higher degrees of protection for each higher classification level (Confidential, Secret, Top Secret). A rigorous operations security program helps management identify threats and mitigation measures. The operations security activities at Pacific Northwest National Laboratory directly relate to and support counterintelligence program initiatives.

5.5.5 Counterintelligence

The Laboratory's National Security Directorate has implemented an effective and proactive Counterintelligence (CI) Program that closely coordinates its operational elements with their counterparts in Safeguards and Security Services. The essential mission of this CI Program, as defined from a national perspective, is to conduct activities to protect DOE/NNSA classified and sensitive programs and information, personnel, and assets from foreign intelligence collection and international terrorist activities; and to detect and deter trusted insiders who would engage in activities on behalf of a foreign intelligence service or international terrorist entity. Three over-arching goals articulate the Laboratory's strategy to achieve this mission:

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

In accomplishing these goals, the CI Program executes its responsibilities with recognition of the importance of preserving an open, but appropriate, scientific environment, to include sound management of foreign interactions beneficial to national security interests. The CI Program also complements and supports the Security Program's risk-based approach by countering site-specific threats directed against the Laboratory by foreign controlled adversaries. Certain CI activities result in the development of information that can be evaluated and used to provide appropriate security measures to protect resources that are known, or suspected to be, targeted by adversaries. CI-developed information also enhances the Laboratory's ability to eliminate unnecessary security procedures and appropriately redirects security systems and processes based on risk. This activity is an integral part of the overall protection program and is a pivotal information-gathering process for identifying actual and potential threats to the Laboratory's activities and information. The Laboratory's Senior Counterintelligence Officer, who also serves as the Director of PNNL's Counterintelligence Program, is an active member of the Integrated Safeguards and Security Senior Management Council.

The CI Program is a balanced and integrated effort focused on the following sub-program areas: analysis and risk assessment, investigations, training / CI awareness, information/special technology coordination, personnel evaluation, and Intelligence Community (IC) support. The CI Program closely coordinates each of these efforts with the FBI, other members of the Intelligence Community, and federal, state and local law enforcement agencies through an aggressive liaison program. Integration into the Laboratory is primarily achieved through CI focused training initiatives that have been developed and implemented to meet program



Information security at the Pacific Northwest National Laboratory involves the securing of classified matter.

objectives in conjunction with the security education and awareness program and Lab-wide communications media. These programs have resulted in close and cooperative relationships between staff participating in DOE international scientific and nonproliferation exchanges and the Counterintelligence Officers.

Additionally, collaborative relationships with Laboratory computer security personnel have been developed. Counterintelligence Officers, who have special technical skills in the computer science field, work with local computer security staff to effectively implement unique cyber projects, such as intrusion detection, suspicious e-mail, and website analysis. Complete and timely responses to DOE Office of Counterintelligence requests for raw intelligence in support of analytical studies is also performed. Both a strategic and tactical CI analytical capability has thus been developed and implemented. This capability provides site-specific threat and vulnerability assessments and other CI/CT analytical products, including those done in conjunction with local Field Intelligence Element personnel to support the research and analysis needs of the IC and DOE.

5.5.6 Cooperative Research and Development Agreements and Work for Others

Cooperative research and development agreements and Work for Others programs are primarily protected by the project managers through the operations security, counterintelligence, and information security programs, which are structured to provide management with the necessary information required for sound risk management decisions concerning the protection of information. Notification is received from DOE for approved Work for Others programs. Draft statements of work are received prior to commencement of cooperative research and development agreements. Results of operations security assessments, counterintelligence and foreign national activities coordinator reviews, export control and technology transfer reviews, as well as scientific and technical subject matter expert reviews are analyzed and, in consonance with risk management, countermeasures are developed and implemented, as appropriate.

5.5.7 Personnel Security Program

Among the more than 3,700 staff at Pacific Northwest National Laboratory, approximately 1,100 possess security clearances. Our personnel security program ensures that individuals are processed for, granted, and retain a DOE access authorization (clearance) only when their official duties require such access. The program maintains the minimum levels and numbers of clearances necessary to ensure the operational efficiency of DOE programs and operations.

Staff Protection and Visitor Control

We protect our on-site and off-site staff using access control systems, administrative procedures, and other security measures implemented in a graded manner. These measures are documented through asset protection agreements and/or security plans for all facilities (both on-site and off-site). They take into account the nature of the security interest, protection requirements, threat potentials and countermeasures, and assign a safeguards priority position based on a composite evaluation of these factors.

We provide visitor control by maintaining procedures for processing visits to and from Pacific Northwest National Laboratory so that only officially authorized visitors are permitted access to classified or sensitive information, materials, or areas. Incoming visits of U.S. citizens and foreign national visits and assignments, as well as outgoing visits of staff to other locations, are coordinated, processed, and tracked. Individuals traveling abroad coordinate the travel through Safeguards and Security (Foreign Travel Office) and the Counterintelligence Office. Recent implementation of a Foreign Travel Request web application system has significantly improved this process. This new automated system replaces the manual paper process, incorporating the Laboratory's electronic signature application.

Our review process ensures foreign national visit and assignment activities (including hiring) are coordinated and reviewed from an integrated perspective to determine the overall need and associated benefit. Operations security, counterintelligence, export control liaison, and the Laboratory approval authority receive information regarding all foreign national visits, assignments, and hire requests. The Laboratory utilizes an automated request system for processing foreign national visits and assignments. System enhancements implemented during the past year included a new web-based entry system, and automated e-mail reminders, and promotes the next phase of importing/exporting data between the Laboratory and DOE systems. These enhancements also have resulted in the simplification and streamlining of associated administrative activities.

During fiscal year 2001, there were over 6,800 visitors to the Laboratory. Over 350 of these visits involved classified interactions and over 670 were for foreign national visitors and assignees.

5.5.8 Cyber Security

Cyber security at the Pacific Northwest National Laboratory includes all personnel, operating equipment, and maintenance activities associated with unclassified (both sensitive and nonsensitive) and classified information and information systems, and cyber infrastructure. The strengthening of our cyber security program is an ongoing priority for the Laboratory. To support this priority, the Laboratory pursues timely implementation of cyber security solutions and constantly evaluates emerging technologies and the potential applications that may be useful in this area. The Laboratory has made great strides in strengthening cyber security as emphasized by the Hamre report in this area. One primary factor was the transfer of the budget and responsibility for computer (cyber) security from the Information Technology organization to the Safeguards and Security activity. Additionally, a formal risk assessment process is implemented for all computer systems that results in the identification of a level of protection for these resources based on the level of risk involved.

The unclassified computer security program is responsible for the policy, guidance, and strategies for the protection of all unclassified information and information systems that generate, receive, transmit, use, store, reproduce, or destroy information in electronic form. The protection level for information and systems is commensurate with the threat, risk, and potential harm that could result from the loss, misuse, disclosure, or unauthorized modification of information processed, stored, or transmitted by electronic methods. Protection includes all security-related



The cyber security program at Pacific Northwest National Laboratory ensures the protection of information that is stored, processed, or viewed by electronic means.

activities associated with network management, Internet access, training and education, intrusion detection, system recovery, and cyber security architecture.

A current initiative supporting the Laboratory functioning as a multiple-discipline laboratory is the Environmental Molecular Science Laboratory (EMSL) enclave project. The design of the network enclaves to enhance our security supporting multiple security profiles has been under development for approximately two years. During this time the network resources have been in the process of realignment in order to facilitate the uncoupling of network segments such as EMSL from the rest of the network. The infrastructure to accomplish this is now in place. The next steps will involve modification or duplication of applications that will need to be accessed in both enclaves. This work is being done as the need arises and is an evolving process. Additional funding will need to be available in order to make this a production environment. Implementation of the enclaves will segregate and strengthen the infrastructure to protect the Laboratory's sensitive and classified activities while permitting an open environment for research associated with EMSL.

The classified computer security program is the classified version of our unclassified computer security program. Our key objective is to protect classified information that is created, stored, processed, viewed, or prepared for transmission by electronic means.

5.5.9 Communications Security

In addition to classified and unclassified computer security, the Laboratory maintains an effective communications security program to protect information that must be transmitted by electronic means over telecommunications facilities both internal and external to the perimeter protection boundary of the Laboratory. This includes methods for ensuring the authentication, integrity, and confidentiality of information sent and received between systems and users. The Laboratory was one of the first communication security accounts nationally to implement the newest encryption technology, Secure Terminal Equipment.



The Laboratory's effective Communications Security Program protects information that must be transmitted by electronic means both internal and external to the Laboratory's perimeter protection boundary.

Cyber infrastructure protection includes all operations and maintenance for protecting computer and information systems critical to facility operations from traditional and information warfare threats (both internal and external adversaries). Computer and information systems critical to the maintenance of the infrastructure include automated process control systems; fire, criticality, and security alarm systems; telephone and network switching systems; electrical power distribution control

systems; oil and gas distribution control systems; and other supervisory control and data acquisition systems.

5.5.10 Export Control

The export control program protects U.S. government-controlled and sensitive information. The unauthorized release or access to such information has the potential to undermine the national security and economy of the United States. This proactive program promotes awareness of the various threats to such information and material and institutes essential procedures to minimize risk.

Particular emphasis is placed on precluding access of export-controlled information to foreign visitors and assignees to the Laboratory.

The export control program is founded upon federal regulations that control the transfer of equipment, materials, and information that could adversely affect non-proliferation, national security, and the economic interests of the nation. Elements that the export control program handles for the Laboratory include the following:

- coordination with Counterintelligence, Safeguards and Security, Intellectual Property, Computer Security, Property Disposal, and others as appropriate
- upper level management briefings
- direct linkage with staff involved with overseas programs and travel
- direct linkage with staff hosting foreign visitors and assignees
- ongoing coordination with DOE to identify emerging export control issues.

5.5.11 Program Changes

As a result of evaluations and reviews of projected business involving classified work, Facilities and Operations in conjunction with the National Security Directorate has initiated a Limited Area Island deployment plan for the National Security Building. This activity permits the Laboratory to conduct work with distinction, fully supportive of and integrated with the Laboratory's science and technology mission in the area of national security. It contributes to the operation and maintenance of an optimum set of facilities and supporting infrastructure that are aligned with current and future mission needs associated with classified work. Implementation of the consolidation of classified activities puts the Laboratory in accord with the strategies and requirements of major clients.

The safeguards and security program was funded directly from the Office of Security and Emergency Operations (through the Office of Environmental Management) in fiscal year 2002. The direct funding received was \$10.8 million for our base safeguards and security program. This funding level did not address new or modified requirements that were levied after the baseline budget activity was concluded. Each new requirement requiring additional cost to implement is evaluated and project change requests are initiated if necessary. Guidance from the Office of Environmental Management for future years suggests that our budget will remain constant at ~\$10.5 million. Level funding will make it difficult to comply with all requirements and there are concerns with the lack of adequate funding for the base program (no escalation provided) in future years as well as for emerging safeguards and security requirements.

Funding for maintenance of the Laboratory's safeguards and security program supporting the Laboratory's mission areas may better fit the Office of Science security and safeguards funding allocation process. A recommendation to transfer this funding from the Office of Environmental Management to the Office of Science is currently being discussed by the Laboratory and the Pacific Northwest National Laboratory Site Office.

Our safeguards and security program is responsive to the new requirements, however, our challenge is to balance programmatic needs with the need to achieve

compliance with the security reform measures that are being developed and remain within our approved budget. The Laboratory has been proactive in addressing this challenge through a variety of activities. Innovative approaches and operational efficiencies must continue to be identified to facilitate effective security program performance. The continual maturation of the Integrated Safeguards and Security Management program is one of the most successful activities ensuring appropriate assimilation of current, proposed, and new requirements. Continued integration into the mainstream Laboratory processes is an ongoing strategy of this program.

During fiscal year 2002, the safeguards and security program worked with the Pacific Northwest National Laboratory Site Office and the Office of Science Security Team to develop a separate Security Plan (replacing the Hanford Site Safeguards and Security Plan) for the Laboratory to customize and appropriately document the Laboratory's specific protection strategies consistent with its needs, mission, and to more effectively support research meeting the critical needs of DOE. The Security Plan was approved and now effectively removes the Laboratory from the Hanford Site Safeguards and Security Plan, providing us with an autonomous protection strategy that supports the work and mission of the Laboratory.

5.6 Information Resources

The primary goal of the information resources management program at Pacific Northwest National Laboratory is to provide our staff and collaborators with a best-in-class information technology environment that enables scientific innovation, enhances team and personal productivity, supports effective collaboration, enhances management of the Laboratory's business and assets, adheres to Standards-Based Management System processes, and provides transparent and secure access to information and to scientific and engineering computing resources.

5.6.1 Information Technology Infrastructure

The information technology infrastructure provides the essential networked computer systems and support for all of the research missions at the Laboratory. These resources include computers and computational facilities, systems and databases for scientific and administrative information, network and telecommunications, and user-oriented information services. The infrastructure is specifically designed to support key missions in environmental science, energy science, national security, and fundamental science. Our information technology is focused on four broad strategic computing environments: 1) scientific and technical computing, 2) business information systems, 3) personal computing, and 4) team collaboration and information sharing services. The information environment is implemented using a web-based information delivery model running over a secure, high-performance network infrastructure.

5.6.1.1 Current Capabilities

The network infrastructure has been upgraded to 100 Mb switched Ethernet to the desktop with selective delivery of Gigabit Ethernet services. The network backbone is switched Gigabit Ethernet. The PBX telephone uses a switch capable of supporting voice and data convergence. External connections to the Laboratory now support an OC-3 ESnet link and a backup T1 link to NorthWestNet, a regional Internet service provider. In addition to supporting research programs, projects,

and user facilities at the Laboratory, the OC-3 link also supports the National Science Foundation-funded Laser Interferometer Gravitational-Wave Observatory at the Hanford Site. Remote access to the network now includes high-speed digital subscriber line, cable modem, and fixed-point wireless as well as conventional dial-up services. The internal wireless network pilot program now operates in production status and covers 75 percent of the Laboratory campus with full coverage expected in fiscal year 2003.

Network security has been enhanced in several areas. When the wireless network was moved to production status, it was moved outside the Laboratory firewall and a separate firewall was established between the wireless network and the Internet. Virtual private network encrypted tunnels support remote access. The prototype Public Key Infrastructure initiated in fiscal year 1998 will provide certificates for all staff by the end of fiscal year 2002. The capability to automatically scan for vulnerabilities and install security patches on Windows platforms is now supported. Intrusion detection capability is available at the network perimeter and was installed on key internal aggregation points in fiscal year 2001 and moved into production in fiscal year 2002. A centralized intrusion detection database has also been established to collect and analyze security logs from firewalls, intrusion detectors, and multiple servers.

Business computing for the Laboratory is provided by a networked array of Sun SPARC and clustered Windows 2000 distributed computing systems referred to as the Information Resource Management environment and is piloting Storage Area Network technology and Linux for business applications. This distributed array uses Oracle and Microsoft SQL Server data management software. The Laboratory intranet supports a data warehouse, decision support and business reporting applications, and tracking and reporting systems. We use commercial software to the maximum extent practical for our core applications, which include cost accounting, procurement, human resource management, payroll, travel accounting, facility management, and environment, safety, and health control and reporting. Interfaces to these systems are based on a web-centric, browser-accessible model for enhanced user access and productivity. A role-based access infrastructure is being implemented in fiscal year 2002 and will be integrated with applications in future years.

Desktop computing by our scientists, engineers, and support staff is mainly dependent on standardized Windows operating systems running on Intel platforms. Macintosh systems also are supported at the desktop level, and UNIX platforms are supported for special-purpose and scientific applications. Our computing platforms are acquired through a managed hardware program that features standard hardware and software configurations; pre-configured security settings; on-line ordering; accelerated delivery; and has resulted in reduced acquisition, installation, and maintenance costs. Application software standards adopted as part of this program include Microsoft Office, Exchange/Outlook, Quick View Plus, Netscape, Norton AntiVirus, and Schedule+. Each of these software packages is acquired and maintained under a site license from the vendor.



Current information technology at the Laboratory includes selective delivery of Gigabit Ethernet services.



Staff at the Pacific Northwest National Laboratory have access to a network protected by multiple firewalls.

Supercomputing is available on a high-performance IBM RS/6000 SPJ with 512 processors, an IBM SP with 96-processors, and a 192-processor Dell-Giganet cluster using 500 MHz Pentium 3 processors. In addition, a high-performance visualization and graphics laboratory equipped with advanced Silicon Graphics, Sun, and IBM cluster machines, as well as over 400 high-performance UNIX-based workstations, are available to support the advanced computing needs of our scientific staff.

The Laboratory network is now protected by multiple redundant firewalls. External access to the internal network is enabled for travelers, partners, and collaborators using a combination of protective access measures including SecureID® token access, Virtual Private Network capability, Secure Sockets Layer authentication, and reverse proxy access.

5.6.1.2 Strategies

Our technical strategies for information resources are executed according to the strategic vision described in our Five-Year Information Technology Strategic Plan that is updated every year. Principal outcomes include the following:

- provide, maintain, and operate computing and telecommunications services that enhance individual and group productivity in the conduct of research and the operation of the Laboratory
- effectively integrate and efficiently deploy best-in-class business information systems to enhance research project performance; environment, safety, and health assurance; and management of the Laboratory's business and assets
- design and implement an enclave-based cyber security architecture to support world-class open science while protecting sensitive and classified information and systems
- acquire, develop, and manage Laboratory and client information resources in accordance with good business practices, industry certified processes where appropriate, and applicable laws, regulations, and contractual obligations.

Our external network strategies aim to increase the speed and functionality of existing ESnet connections, and include an upgrade from OC-3 to OC-12 in fiscal year 2003. In future years, we anticipate the need to further increase external network speed and functionality and establish a large-volume mass-storage system to support our strategic vision for expanded user communities and advanced computing, modeling, and simulation.

The internal network transition to switched 100BaseTX Ethernet will be followed by an orderly migration to a Gigabit Ethernet backbone to all major network segments and the delivery of Gigabit Ethernet to selected systems and desktops to support high-performance computing and large file transfers, with up to 50 percent of the desktops Gigabit capable by fiscal year 2006. The wireless network will be expanded to serve most of the campus in the next 2 years. We also will initiate several network convergence activities to support integrated voice and e-mail as well as network videoconferencing to the desktop and selected use of Internet Protocol telephony.

Collaborative computing will focus on providing the capability for virtual collaborations between researchers at remote locations. Capabilities will include both commercial services and software such as WebEx conferencing and commercial off-the-shelf software such as NetMeeting, and custom tools such as CollabraSuite. The Laboratory's infrastructure will support universal and instant messaging, and we will further extend our use of rich media (video, audio, three-dimensional virtual reality).

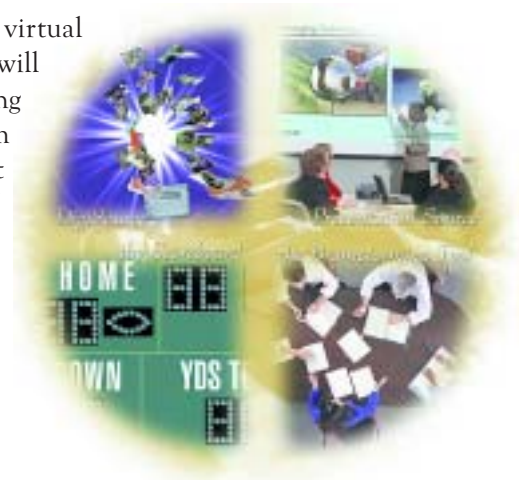
Our strategies for cyber security include

- the design and implementation of a security enclave architecture that moves away from a single protection model for the entire Laboratory to a model that recognizes that each enclave has different assets, risk, access, and protection requirements
- design and implementation of a distributed firewall and intrusion detection architecture
- extending the automated security patching capability to Macintosh, UNIX, and Linux systems
- enhancing the protection of mobile systems like laptops and personal digital assistants
- expanding the analysis capability of the log collection database (intrusion detection, firewall, servers) information with an emphasis on automatic alerts and real-time response
- migrating to IEEE 802.1x port authentication using two-factor token authenticators, and single sign-on for access to the internal network.

Business information systems will convert or build applications to use the role-based authorization infrastructure to provide role-appropriate views of business information. Portal technology will be used to develop role-based information portals and to enable selected business processes to use the enterprise Public Key Infrastructure for integrity and digital signature services. Enterprise tools for document management and unstructured information retrieval support proposal development, good practices sharing and technology commercialization. Depending on the results of fiscal year 2002 pilots, we expect to move the Storage Area network and Linux pilots to production status in fiscal year 2003.

5.6.1.3 Resources and Initiatives

Information technology is pervasive in the Laboratory's work environment and is used by almost every staff member. Consequently, most business information systems and infrastructure enhancement, maintenance, and operation activities are funded from Laboratory-level overhead accounts and general-purpose capital, rather than charge-back to individual cost objectives. Charge-back is used to recover maintenance and operation costs for capabilities and services used by a smaller percentage of the Laboratory. Budgets for both classes of service are reviewed and approved by senior management as part of the annual budget planning and allocation process.



Custom software tools, such as CollabraSuite, enable people from remote locations to collaborate virtually on projects.

5.6.2 Scientific and Technical Information Program

The Laboratory's Scientific and Technical Information program provides guidance, products, and services to support proposal development, intellectual property development, and the communication of research results. The program supports the technical organizations as they seek information important to their research projects and to meet contractual requirements for publication and dissemination of scientific and technical information. In addition, this program will support the life cycle of scientific and technical information, from creation through product development, dissemination, retention, and reuse.

5.6.2.1 Current Capabilities

We provide researchers with desktop access to information tools, such as on-line technical journals and other library resources, and the Electronic Records and Information Capture Architecture (ERICA) system. ERICA enables appropriate review of information for intellectual property and other sensitivities. ERICA also enables the Laboratory to keep pace with current federal and client records requirements, streamlines work processes, and positions the Laboratory to comply with DOE's plan to deliver published scientific and technical information electronically.



Many of the Laboratory's information assets are stored at the Hanford Technical Library.

The Hanford Technical Library is the steward of much of the Laboratory's information assets. The library is located in the Consolidated Information Center, together with the Washington State University Tri-Cities Library and the DOE Public Reading Room. The Technical Library also has a Legal Library branch located in the Federal Building. The Technical Library collection focuses on energy, engineering, environmental sciences, chemistry, life sciences, and other basic sciences. The DOE

Public Reading Room contains reports related to current and historical operations at the Hanford Site. The Legal Library houses legal and regulatory material.

The library continues to aggressively add resources to the desktop via the intranet. Laboratory staff may access the Library's catalog, over 700 full-text journals, and a variety of scientific and bibliographic databases, such as Web of Science and INSPEC, from their desktops.

5.6.2.2 Strategies and Initiatives

A major focus of the Scientific and Technical Information program is on various aspects of information stewardship. The ERICA system architecture has been reworked so that the system can be used to support new internal and external requirements, such as tracking and reporting publications of non-Pacific Northwest National Laboratory staff who conduct work in DOE user facilities such as the Environmental Molecular Sciences Laboratory.

The library will continue to enhance its collection of desktop resources, adding scientific and engineering databases, full-text journals, and other published literature key to the Laboratory's major initiatives. The library will aggressively select and purchase products and technologies that enable seamless linking between databases and the published literature, facilitating access across distinct bodies of

literature. In addition, the Technical Reports collection^(a) (approximately 800,000 items) will be added to the library's on-line catalog, improving access to Pacific Northwest National Laboratory's publicly available technical publications dating back to 1965.

Another key focus of the Scientific and Technical Information program is bibliometrics—the study of the impact of the Laboratory's research publications. Statistical analysis of publication data for the past several years can reveal a “portrait” of the Laboratory's presence in the most influential research journals. Such a portrait can be useful in high-level decision-making about investments to strengthen our reputation in key strategic areas.

5.7 Communications and Trust

Pacific Northwest National Laboratory's goal is to support the Department of Energy in creating community awareness and building trust with key audiences through timely communications, regional involvement, and public awareness. We will continue to provide open and timely communications that build awareness of and advocacy for the Laboratory as a premier science and technology research laboratory.

Our goal is to make significant contributions to local and regional economic development, to science education, and to other major community interests. We unite with various constituencies in the community and Northwest region to build a strong and diverse economy, with particular emphasis on scientific technology development and deployment. Our strategy uses a five-pronged approach:

- expand existing businesses
- start new businesses
- attract outside business to the region
- create a supportive business climate
- enhance the quality of life.

5.7.1 Programmatic Activities

Our current communications and community development activities build on past good relations and form a strong foundation for our efforts in the next 5 years. For the past 3 decades, the Laboratory has been involved in and has invested heavily in our community. Our contributions have ranged from innovative science education programs that expand student and teacher knowledge to donations that support a wide range of health and human services. On average, we invest about \$2.5 million per year of Battelle private funds in the community through communications, economic development, community relations, and education.

(a) Technical Report Files contains reports produced by the Department of Energy, its predecessors, (the Energy Research and Development Administration and the Atomic Energy Commission), and their contractors as well as materials from foreign nuclear energy agencies. In addition, there are significant holdings from the Nuclear Regulatory Commission, and limited holdings from the Department of Defense, Environmental Protection Agency, and the National Aeronautics and Space Administration. The collection is arranged in report number order. Full-sized materials circulate to Hanford and Laboratory staff, while the microfiche collection can be viewed at the library.

- **Communications.** By providing open and timely information, our communications programs enable the Laboratory to create awareness and build trust with key audiences. We will continue to place articles in national, regional, and local media that enhance the Laboratory's scientific and technical reputation. We also will use several electronic tools that provide our customers and the general public with easy access to Laboratory news and information. We will use targeted publications to reach identified audiences.

In the future, we will continue to provide leadership in support of DOE's objective to create awareness and build trust with our neighbors. We will continue to expand information resources at the desktop, enhance Internet-based resources, and strategically contribute meaningful science and technology articles in the mass media to meet this goal.

- **Economic Development.** Through our Economic Development Office, we assisted more than 500 businesses since 1995 and helped create 60 companies in the last 6 years. In the future, we plan to
 - generate new, technology-based companies
 - bundle together intellectual property from the Laboratory and partner with universities to improve commercialization opportunities for regional businesses
 - promote the growth of innovation-driven companies statewide through collaborations between the Applied Processing Engineering Laboratory in Richland, and the Seattle-based Washington Technology Center and the Spokane Intercollegiate Research and Technology Institute. (Pacific Northwest National Laboratory alumni, further demonstrating the Laboratory's influence on technology-driven economic development in the region, currently head all three.)
 - encourage new industry to move into the region by pursuing tax incentive zones.
- **Community Relations.** Many of our community relations efforts are donated from private Battelle funds to support a wide array of programs that enhance the image of both Battelle and Pacific Northwest National Laboratory in the region. One of our most impressive programs is Team Battelle, a Battelle-funded program designed to recognize and support staff members who volunteer in the community. Now entering its fourth year, Team Battelle volunteers logged more than 20,500 hours in 63 community projects in fiscal year 2001. Projects ranged from painting the handicap ramp at the Lourdes Wilson House, to being the top community fundraiser for both the Junior Achievement Bowl-a-Thon and the Neurological Center's Alzheimers' Walk/Run. Another successful community relations program is our Speakers Bureau, which relies on staff volunteers to make presentations about science and technology to local and regional organizations.



Pacific Northwest National Laboratory's Economic Development Program provides technical assistance to businesses, such as Mobility Engineering, which designs and manufactures vehicles for the physically impaired.

In addition to Team Battelle and Speakers Bureau, we operate a Corporate Contributions program that supports projects providing lasting benefits to the community. Among the recipients of the more than \$730,000 we donated in fiscal year 2001 were the Safe Harbor Nursery, Academy of Children's Theatre, Heritage College, and five school districts that partnered with us for scientist/student/teacher research projects.

In the future, we will continue to enhance community development by expanding the Speakers Bureau, building on the success of Team Battelle, and implementing activities that support the Laboratory's efforts to link with local minority communities. We also will continue to work with community leaders and decision-makers to develop broad impact projects that improve the quality of life in the Tri-Cities and the region. Pacific Northwest National Laboratory's involvement in the community is coordinated by the new Community Involvement Council.

- **Science Education.** Our nation's future is inextricably linked to developments in science, mathematics, and technology. The demands of our changing economy and workplace, the need for an educated citizenry, impact on our national security, and the intrinsic value of mathematics and scientific knowledge make these areas essential to the education of today's students for tomorrow's world. For that reason, the Laboratory is committed to supporting science and engineering education from grade school through graduate school.

The Laboratory's science and engineering education programs are key to enhancing the Laboratory's value to our community, region, and nation. We promote science education through strategic goals centered around leadership in science education reform, education and mentoring of future scientists, and diversity in the science and engineering pipeline. Our programs span kindergarten through postdoctoral education. Although the programs vary with the different age groups, the themes of these programs are closely tied to our strategic goals. Last year, through Laboratory-sponsored programs, more than 3,000 students and teachers experienced, first-hand, the excitement of science and technology.

A primary emphasis in our kindergarten through 12th grade programs is on science education reform. These programs support teacher development, student internships, and curriculum enhancement. Although these programs are mostly implemented at the regional and state level, our efforts have received national attention.

The Laboratory spearheaded the growth of the Washington State Leadership and the Assistance for Science Education Reform (LASER) project. We co-lead this state project with the Pacific Science Center in Seattle. Fifty-five Washington school districts serving 166,000 students participate in this project. Washington LASER is affiliated with the National Science Resources Center's National LASER Project. National Science Resources Center's parent organizations are the prestigious National Academies and the Smithsonian Institution.

In our Partnership for Arid Lands teacher project, we provide professional development for elementary teachers as part of an environmental science education and research initiative focused on the arid lands of the Columbia Basin. Teachers from around the region take part in field-based research scenarios designed to build their content knowledge and skills in the ecological sciences. A teacher's handbook, website, and reference book on the terrestrial



As Team Battelle begins its fifth year at PNNL, employees continue to expand their volunteer support into more areas of need, positively impacting the quality of life in our community.



The Laboratory's Partnership for Arid Lands teacher project provides field experience for regional teachers in the area of environmental science.

ecology, aquatic ecology, geology, and cultural resources of the Columbia Basin enhance both formal and informal environmental science education in the region.

At the elementary level we sponsor a Family Math and Science program that trains teachers, parents, and community members to successfully conduct Family Math/Science programs in their schools and community. This program builds community support and understanding for quality mathematics and science instruction in schools.

Our Teacher Research Participation program is focused on high school and community college faculty who teach science, mathematics, and technology. The faculty receive summer research appointments at the Laboratory and work side-by-side with our research scientists. Also at the high-school level we sponsor, with the University of Washington, a Materials Science and Technology workshop that prepares secondary school teachers to teach materials science and technology in the classroom.

Through a Department of Energy/National Science Foundation program, we sponsor undergraduate preservice teachers during the summer at the Laboratory. This program is also aimed at reforming how science is taught in our schools. The preservice teachers are exposed to laboratory-based scientific research and use this experience to develop classroom curricula that they may use as future science teachers.

The Laboratory also plays an important role in educating and mentoring future scientists and engineers. This strategic goal primarily focuses on high school and undergraduate students. The Department of Energy sponsors the largest programs—the Energy Research Undergraduate Laboratory Fellowships (ERULF) and the Community Colleges Institute. The Office of Science ERULF program provides academic-year and summer research appointments to undergraduates in science, mathematics, engineering, and technology fields of study. The Community Colleges Institute provides summer research appointments to community college students in the fields of biotechnology, computer sciences, and environmental sciences. Laboratory research programs also sponsor hundreds of summer undergraduate and graduate students through the Laboratory Co-Operative Program.

The predicted shortages in science and engineers must be addressed today by promoting diversity in the science and engineering education pipeline. To this end, the Laboratory is involved with several programs. The Mathematics, Engineering, and Science Achievement (MESA) Partnership is between the Yakima Valley/Tri-Cities and the Laboratory and is designed to increase the number of underrepresented minorities in these technical professions. The partnership targets kindergarten through high school students and provides participants with educational enrichment experiences and practical help to prepare for university-level studies in these fields. At the high school level the Laboratory sponsors the Student Research Apprenticeship Program, which targets high school students historically underrepresented in mathematics, engineering, and science. Students receive summer research appointments at the Laboratory and take part in academic follow-up activities.

At the college level, DOE sponsors the Faculty and Student Teams (FaST) Fellowships, a partnership with the National Science Foundation. This program provides faculty/student teams from historically black colleges and universities and other minority serving institutions (e.g., Hispanic and Native American) with summer research appointments in science, mathematics, engineering and technology fields of study.

We strive to maximize the impact that our education programs have on the future science workforce. Last year, approximately 110 college students and faculty were funded through DOE's education programs. An additional 600 college students and faculty were funded directly by individual research projects and education programs at the Laboratory. The Office of Science-supported research at the Laboratory makes significant impact on the training and education of future scientists and science educators (see Table 5.3).

We believe that we achieve heightened community trust achieved by the contributions we make to a better society. This Laboratory will continue to support our region's economy by nurturing a business climate that encourages businesses to grow and thrive in our community. We plan to support this growth by strengthening our research and development base with new initiatives in the biological and information sciences, health, materials, energy, and the environment.

In the future, the Laboratory's role will expand as we help shape and energize the region's economy and advance our quality of life. With a strong and diverse community, current businesses will prosper, new businesses will move into the area, and population growth will be sustained. As a result, Pacific Northwest National Laboratory will be in a strong position to attract and retain the best and the brightest people to the Laboratory. These efforts will protect and enhance the value of our infrastructure, will foster an environment for growth and diversity, and will continue to generate the goodwill that we are best known for in our community.



The Faculty and Student Teams (FaST) program is a DOE partnership with the National Science Foundation. This program provides scientific research appointments to faculty and students at institutions with programs for under-represented students.

Table 5.3. University and Science Education

	FY 2002			FY 2003 Estimated		
	Total	Minorities	Women	Total	Minorities	Women
Pre-College Programs						
Student Programs						
Student Research Apprenticeship Programs	12	12	10	12	12	10
Student Research Internship Program	39	3	14	40	3	15
DOE Science Bowl Competition ^(a)	180			180		
DOE Science Bowl Workshop ^(b)						
Young Women in Science	5	2	5	5	2	5
Mathematics, Engineering and Science Achievement (MESA)	739			740		
Teacher Programs						
Teacher Research Participation Program	6	0	2	6	0	2
Partnership for Arid Lands Stewardship	46	0	45	45	2	40
Washington State Leadership and Assistance for Science Education Reform Events ^(a)	654			654		
DOE Science Bowl Competition ^(a)	36			36		
Materials Science and Technology Workshop ^(a)	200		0	200		
Family Math/Science Workshop ^(a)	37			37		
Undergraduate Programs						
Office of Science Undergraduate Laboratory Fellowship (SULL, formerly called ERULF)	49	7	26	50	8	25
OFP Fellows Program	224	20	79	225	25	80
Community College Institute	23	10	8	25	11	10
OFP Limited Term Employees						
Pre-Service Teacher Program	15	3	10	15	2	9
Mickey Leland Undergraduate/Graduate Fellowships	7	2	6	7	7	3
Faculty Student Teams (FaST)	9	2	3	10	3	4
Graduate Programs						
OFP Fellows Program	52	13	25	60	15	30
OFP Limited Term Employees	20	3	6	25	10	15
Postgraduate Programs						
Post-Baccalaureate Program	35	6	19	35	8	20
Post-Masters Program	22	5	7	25	5	10
Postdoctoral Program	104	45	20	110	40	30
Faculty Fellowships	21	8	5	25	8	7
Faculty Travel Grants	2	0	0	2	0	0
Faculty Sabbatical	2	0	0	3	0	1
Visiting Scientists	13	4	3	10	4	3
Other Programs						
Sharing Science with Schools ^(a)	2,153			2,100		
Shadowing Program ^(a)	53			50		
Family Math Programs ^(a)	37			37		
Bridges Program	14	1	4	15	2	5

(a) Data on minorities and women are not tracked for these programs.

(b) PNNL did not participate in this program in FY 2002, but may participate in FY 2003.

Site and Facilities Management

The Pacific Northwest National Laboratory of today offers a unique research environment designed to house state-of-the-art laboratories and equipment that our research staff members use to meet the needs of our global research agenda and the interests of our collaborators. The Richland-North campus, which is our core location, has the look and feel of a modern high-technology scientific research center in a modern university setting. Top scientists (permanent staff, users, and visitors) are drawn to the campus because of the research capabilities, opportunities for collaborations, a reputation for world-class science and technology, and visitor-friendly facilities.

The Pacific Northwest National Laboratory of tomorrow, and the facilities, resources, and capabilities in support of the PNNL 2010 vision, will focus on key research areas. As described in the May 2002 Genomes to Life “DOE Resources and Technology Centers for Biological Discovery in the 21st Century” report, DOE requires new and enhanced technical resources to address a new era in biological sciences and its application—the age of systems biology. These new facilities and resources will build on and extend the William R. Wiley Environmental Molecular Sciences Laboratory’s unique capabilities in supporting DOE’s advanced systems biology needs. User community access to mass spectrometry, nuclear magnetic resonance spectrometers, and other one-of-a-kind research instruments will advance the understanding of functioning cells and organisms and their interaction with the environment. Facilities and resources with high-throughput protein production and expression capability will allow the development of new sample separation and preparation technology, instrumentation development, mass spectrometry analysis, and integrated bioinformatics and computation.

The Computational Sciences investment area recognizes that laboratory scientists conduct ever-increasing computations and simulations as an alternative to bench-level experimentation. Existing supercomputer resources have not kept pace with either the demand for high-performance computing or the current state of technology. High network bandwidth is needed between graphics and visualization laboratories, workstations, and computing resources. The PNNL 2010 vision sees the computational capability as an investment in the future, and as a result, the strategic roadmap includes a new facility to house these capabilities, with the specialized systems in place to accommodate a data-intensive laboratory environment. High-performance computing, together with the collocation of the Computational Sciences and Mathematics staff will ultimately maximize collaborative research opportunities.

Prior to the events of September 11, 2001, the PNNL 2010 vision recognized the National Security Directorate as a major investment area. In light of the international climate today, security-related research has become an even more critical focus area. As a result of specific facility infrastructure investments and collocation of staff, the National Security Directorate has realized a dedicated facility. As the National Security Program continues to expand, additional

Our goal is to provide an infrastructure that promotes seamless collaborations in the development and commercial deployment of important new intellectual assets. Our facilities must enable scientific and technical achievements and collaborations with large teams of researchers.

collocation of resources will be achieved to support the Directorate's mission to develop innovative solutions to critical national and international problems by applying and deploying the full science and technology capabilities of the Laboratory to our safety and security programs.

Pacific Northwest National Laboratory's continued involvement in agricultural and bio-products research has established the Laboratory as a leader in delivering solutions to the agricultural industry. The hallmark of our research is expertise in the area of chemical and biological processes, converting low-value or waste biomass into industrial and consumer products, fuels, and energy. The Bio-Products Research Facility represents a collaborative partnership with the Washington State University whereby a facility will be designed and built to accommodate Laboratory research as well as university staff, students, and visitors.

Projected global energy demand will challenge the nation's economic well-being and pose a significant impact on the environment and national security. Nuclear science and technology has a role in finding solutions that will meet global demand in an environmentally sound and sustainable way. Innovative research leads to technology discoveries, addresses safety and nuclear material proliferation concerns, and removes barriers to maintaining current nuclear capabilities and also the future use of the nuclear option in the energy, medical, and national security fields. Existing 300 Area facilities and equipment provide the resources and focus for teaming with universities to assess, refocus, and reinvigorate nuclear science and industrial technical capability.

As research areas continue to focus on the future, the Laboratory must focus on future requirements relative to facilities and equipment. Implementation of the PNNL 2010 vision is intended to align facilities and infrastructure strategies with the major research investment areas. Facilities strategic plans, although focused, shall be as dynamic and flexible as the research they support.

6.1 Laboratory Site and Facilities

The facilities that make up the Pacific Northwest National Laboratory have evolved from Hanford laboratories and the original set of buildings that Battelle began constructing in 1965 in Richland, Washington. These Laboratory holdings include facilities that are owned by the U.S. Department of Energy and buildings that are owned by Battelle or leased from others. Through a formal arrangement with DOE, this collection of DOE and privately owned facilities makes up the consolidated Laboratory that is home to more than 3700 scientists, engineers, and support staff. These facilities support advanced scientific research for DOE, other federal agencies, and industry. Increasingly, these facilities also support a wide range of other occupants, including visitors, users, scholars, collaborators, students, and others.

The Laboratory has 183,000 square meters (1,965,000 square feet) of facilities (see Table 6.1, FY 2002 Laboratory Space Distribution). As identified in this table, 46 percent of Pacific Northwest National Laboratory facility space is in DOE-owned buildings located at the south end of the 300 Area on the Hanford Site. The Department of Energy's Richland Operations Office proposal for restoring the Columbia River corridor completes cleanup of the 300 Area in the year 2012. Except for the Environmental Molecular Science Laboratory, it is not clear which 300 Area buildings will remain operational for PNNL future use.

The Environmental Molecular Sciences Laboratory and DOE-leased buildings are located just south of the 300 Area close to the Battelle privately owned and leased buildings. The remaining Battelle privately owned buildings are located at the Marine Sciences Laboratory in Sequim, in northwestern Washington State.

Each cluster of facilities uses different utility service providers. The Project Hanford Management Contractor and Johnson Controls, Inc., provide utility services to the 300 Area DOE-owned facilities. Facilities outside the 300 Area obtain utilities and services from the local municipality. The 300 Area utility and service costs are prorated to area occupants. As the other Hanford Site contractors exit the area, the Laboratory will assume more of the total cost. Pacific Northwest National Laboratory continues to work with the DOE Richland Operations Office and the Hanford Site Integrated Group to ensure that the Laboratory’s physical plant requirements are supported beyond the end of the current environmental restoration era at the Hanford Site. Transition to City of Richland utilities and services is proposed in parallel with the River Corridor cleanup activities.

The majority of the DOE-owned active buildings are 1950s vintage, with an average age of 34 years (excluding the new Environmental Molecular Sciences Laboratory) (see Figure 6.1). Laboratory buildings require considerable investments to support world-class research (see Figures 6.2 and 6.3). The majority of Battelle privately owned buildings are 25 to 37 years in age. These aging facilities also require major capital investments to continue to meet DOE missions at the Laboratory. Battelle Memorial Institute provides capital improvements for Battelle-owned buildings.

Pacific Northwest National Laboratory has developed building life cycle plans for each building. The building life cycle plans are updated as new information is made available and are revised periodically as building walkthroughs are conducted every 3 years. Building maintenance and operations annual work plans are written as part of the planning and budget process. The work plans detail predictive, preventive, and planned maintenance activities, along with an estimated level of corrective maintenance effort. The building life cycle plans, the list of deferred maintenance items, and programmatic capability needs determine the replacement and rehabilitation investments priorities for each building.

Table 6.2 summarizes the present value of the Laboratory’s active buildings. The DOE replacement value for fiscal year 2002 is \$411 million. The Battelle-owned building replacement value is \$99 million (using the DOE methodology).

Location	Area Square Feet (Million)	Square Meters (Million)
DOE Main Site (300 Area)	0.901	0.083
DOE Leased	0.076	0.007
Battelle Main Site (Richland)	0.451	0.042
Battelle Sequim	0.045	0.004
Battelle Leased	0.509	0.047
Total	1.965	0.183

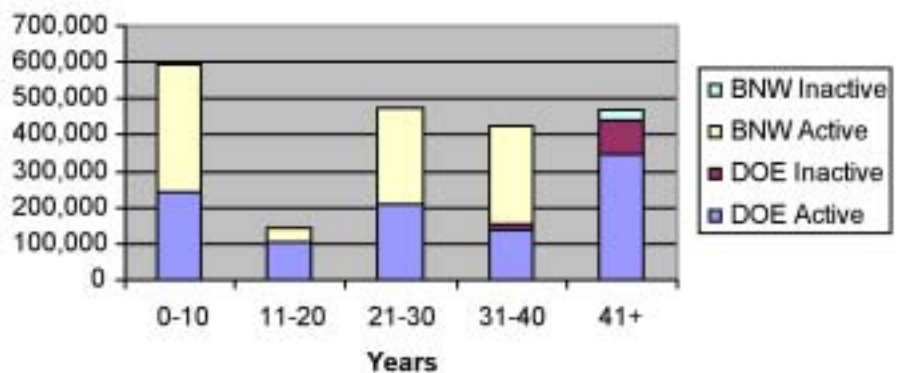


Figure 6.1. Age of Laboratory Buildings

Table 6.2. Facility Replacement Value

Active Facility	Replacement in Current \$M
DOE-Owned Total	411
Battelle-Owned Total	99

The condition of the Laboratory’s general plant equipment is fair. Fabrication and maintenance shops have over 65 pieces of major equipment, much of which was acquired during the 1950s, 1960s, and 1970s. This dated equipment presents a variety of problems such as inability to hold tolerances, hard-to-find replacement parts, and few factory-installed safety and computer-aided features. Recent acquisitions in electric discharge machining and percussion cutting (water jet) has helped the shop to keep pace with research needs, but replacement of outdated equipment is needed to ensure accurate, efficient fabrication and maintenance, and worker safety. The Pacific Northwest National Laboratory computer network infrastructure is continually upgraded to meet the ever-increasing research demands. A graded approach to system upgrades ensures critical needs are being met; however, pockets of technical obsolescence remain a threat.

6.2 Laboratory Site and Facility Trends

6.2.1 Consolidation and Renewal

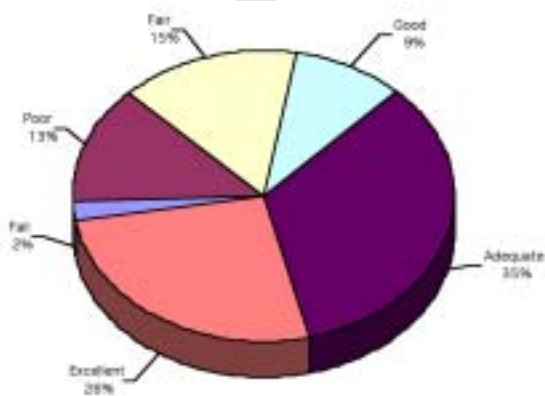


Figure 6.2. Condition of DOE-owned Laboratory space

Pacific Northwest National Laboratory is in the final stages of a facility consolidation strategy started in 1995 to improve the condition and use of space and to reduce the cost of operations. Buildings and structures whose age and condition did not support the investment needed for rehabilitation were vacated. Mission-critical research and support activities were moved to a core set of buildings. Disposition of 90 DOE (389,365 gross square feet) and 13 Battelle (43,331 gross square feet) facilities was completed. This included 27 DOE and 10 Battelle trailers. Only one DOE and two Battelle trailers remain in use. All but one off-site lease was canceled and staff moved to on-site facilities.

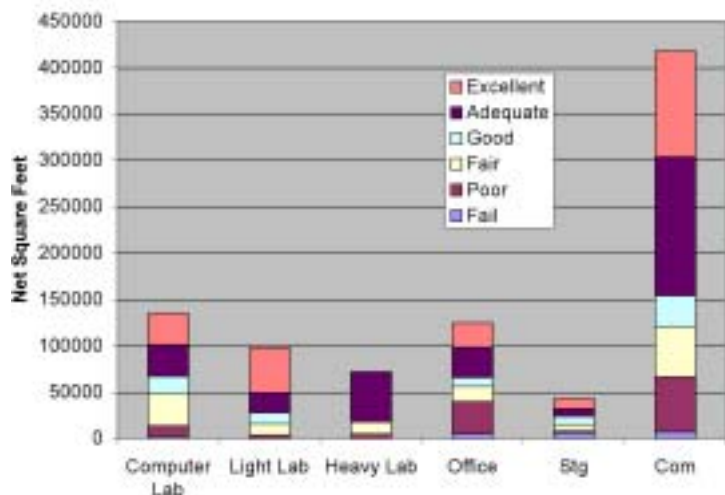


Figure 6.3. Use and Condition of Active DOE-owned Laboratory space

Planned maintenance and rehabilitation investments are restricted to mission-critical buildings. New facility capabilities have been acquired through alternative financing strategies. A total of 350,294 gross square feet of office and laboratory capability have been added through third-party financed build-to-lease arrangements.

6.2.2 Improved Maintenance and Operations

The condition, maintenance, and operations of the physical plant have improved through self-assessment, benchmarking, and implementation of lessons learned. The strategy of consolidating research activities into a core set of facilities and

improved work practices have generated an accumulative cost savings and cost avoidance of \$80 million in maintenance and operations since 1995. These savings have not been at the expense of building condition or system reliability. Metrics monitoring performance of critical systems indicates high reliability. Space deemed in adequate condition has increased by 23 percent since 1995, while space requiring minor or major rehabilitation has decreased by 21 percent. Space requiring replacement has decreased 2 percent. The backlog of deferred maintenance shows a slight decrease. The actual 2002 maintenance investment including capital expenditures was \$11.4 million, 2.8 percent of replacement value.

Proposed initiatives to further improve work practices include field deployment of handheld computers and laptops to create paperless access to maintenance databases, establishment of a system performance monitoring and analysis process to move away from the cost of a traditional “time based” preventive maintenance programs, and use of a maintenance investment model that allows a comparison of actual facility maintenance investments against an idealized life cycle profile from industry (via benchmarking).

Even with these improvements, at times the accomplishment of the Laboratory’s missions is negatively affected by the condition of general purpose infrastructure and unfunded maintenance backlog. The condition of the 320 Building is poor with a deferred maintenance backlog of \$8.8 million. Research programs experience inefficiencies and rework to compensate for poor building climate and air control, quality of water, building system reliability and general building architectural condition. Line item funds to rehabilitate or replace this 37-year-old building infrastructure have been requested. The 3720 Building is located at the north end of the 300 Area within the cleanup zone. Its condition is rated fair with a deferred maintenance backlog of \$2.3 million. The lack of funds to relocate research activities out of the 3720 Building and other 300 Area buildings increases operational risk and compels continued building maintenance and repair investments.

6.2.3 Partnering to Expand Capability

High-performance research equipment and complex, intricate research methodologies require equally complex, high-performance facilities. Humidity, temperature, and vibration control, along with air, water, and electrical quality are increasingly important. Efficient use of space and equipment, and facility configurations that attract, retain, and enable staff to do high-value research is vitally important. Acquisition, rather than renovation of existing facilities, is often the most cost-effective approach to capability development. Through collaborations and the use of alternative financing methods, Pacific Northwest National Laboratory has been successful in obtaining new facility capabilities. By partnering with local government entities, a state-of-the-art laboratory incubator facility with environmental waste discharge permits was created for technology development and demonstration. The PNNL 2010 vision for the campus will require the support of federal, state, and local government; industry; and other stakeholders, along with DOE’s continued willingness to use innovative acquisition strategies.

6.3 Summary of 10-Year Infrastructure Plans

The Laboratory has consolidated the majority of its research activities into a core set of mission-critical facilities. The number of DOE and Battelle-owned and leased buildings, trailers, and other structures has been reduced from 185 to 112. The Facility Transition Program completed the disposition of 103 buildings and structures, approximately 432,696 gross square feet, at little or no cost to the Office of Science or government.

- Thirty-five office trailers and small utility buildings were sold as surplus with the buyer paying the cost of removal.
- Thirteen off-site leases were canceled with excess furnishings dispositioned in place.
- Seventeen facilities were transferred to other government contractors for use.
- The Office of Science funded the demolition of five buildings and structures at a cost of less \$1 million.
- Battelle funded the demolition of one office building.
- Thirty-three facilities/structures (141,504 square feet) were transferred for final disposal/demolition.

With the September 2002 transfer of 23 excess facilities to the Office of Environmental Management and the completion of an on-going Science Laboratories Infrastructure project, the final disposition of all currently excessed Pacific Northwest National Laboratory buildings and structures is completed.

Pacific Northwest National Laboratory predicts growth in several key science and technology areas, including the molecular and cellular life sciences, advanced energy and material sciences, computational sciences and system support, chemical process science, and national security programs (including management of classified information). Current planning data project moderate business growth in these mission areas, as well as shifts in both sector and technical network workload mixes. The Laboratory anticipates using a combined approach of renovating existing laboratories, replacing decommissioned laboratories and building new laboratories to meet our need for expanded and modernized research facilities.

6.4 Facility Modernization and Revitalization Plans and Options

6.4.1 Modernization

Pacific Northwest National Laboratory is working hard to keep up with the rapid pace and changing nature of research and development to ensure that Laboratory capabilities maintain pace with the expectations and needs of DOE science missions. As a DOE multiprogram national laboratory, our roles and responsibilities are aligned with the priorities identified in DOE's strategic planning documents and in DOE's research and development portfolio for science, environmental quality, national security, and energy resources. We believe that facility resources will need to expand and change to meet growth and capability requirements to support all of the DOE science and technology mission areas in

Physical plant upgrades and new equipment will be needed as the Laboratory develops scientific capabilities and responds to DOE mission needs through strategic initiatives, research programs, and partnership activities.

the 21st century. An adequate and reliable infrastructure and equipment funding base is required to provide the stewardship that will modernize and maintain the needed physical plant and equipment capability.

Emerging sciences, such as proteomics and nanotechnology, fuel cell technology, chemical processing, and information management, will require new and larger facility configurations, highly specialized instruments, and advanced computer systems beyond that which we currently have in place. Table 6.3 summarizes the investments that will be needed to support Laboratory missions. These investments, whether through modernization or revitalization, will

- provide the quality of working environments that attract and retain high-quality staff
- provide secure computing and laboratory space for classified and national security projects
- address elements of environment, safety, and health that are required to make the Laboratory a safe place for staff, visitors, and the community in which we operate.

In addition, the changing way in which research is conducted is going to continue to challenge the Laboratory's facility infrastructure. For example, we are experiencing an increasing demand to support ever-growing collaborative working environments. The Advanced Nuclear Science and Technology initiative, described in the Major Laboratory Initiatives section of this Institutional Plan, is an example of a facility concept that not only addresses our ongoing mission in nuclear science and technology, but recognizes the growing role collaboration will play in providing a sustainable national technical capability in nuclear sciences well into this century.

Critical to meeting the challenges of modern science is the need to provide increasing computational capabilities. Our PNNL 2010 vision planning identified the need for an enhanced information technology at Pacific Northwest National Laboratory for high-end communication and computing to enable virtual team collaboration and educational partnership opportunities with various academic institutions worldwide.

A facility modernization roadmap has been developed, as well as schedules for adding new facilities and resources to the Laboratory campus.

6.4.2 Revitalization

Today's research equipment and needs for work process flow require substantially different laboratory configurations and services than laboratories of 30 and 50 years ago. Researchers and their ability to conduct work are adversely affected by deteriorating space. The revitalization effort at Pacific Northwest National Laboratory began over a decade ago and substantial progress has been made. Prior facility investments focused on rehabilitating the existing physical plant and reducing occupational safety and environmental risks. These past investments total \$111 million and have placed the Laboratory in a positive position to be the model for DOE laboratories. However, more work must be done to complete our vision and modernize our existing facilities to meet current and future needs. This vision encompasses the entire portfolio relating to work for the DOE Office of Science and for Environmental Management, among others. The project

Our facility plans are designed to encourage and enable Pacific Northwest National Laboratory to be among the world's truly premier scientific laboratories for solving the most critical scientific and technological problems.

Table 6.3. Summary of Investments Needed to Support Laboratory Missions

Investment Area	Mission Support
Systems biology research centers: capabilities, resources, and facilities	Systems biology research centers consisting of new and enhanced capabilities, resources, and facilities are needed to address a new era in biological sciences and its application to DOE missions. Pacific Northwest National Laboratory intends to submit research center proposals in support of the Genomes to Life program and its technical resource requirements as described in the May 2002 Genomes to Life “DOE Resources and Technology Centers for Biological Discovery in the 21 st Century” report. Potential centers would address proteomics, microbial cell dynamics, imaging, computational biology, structural biology, and provide other capabilities, resources, and facilities deemed required to provide an integrated systems biology program engaged in cutting-edge research. These research centers, along with the investment in the multidisciplinary, collaborative research program that integrates molecular biology, biochemistry, physics, mathematics, and computer science, places Pacific Northwest National Laboratory in a position to advance the understanding of complex biological systems in the post-genomic era and meet the DOE Genomes to Life program and other biological sciences needs. As an example, in the proteomics area, a potential Production Proteomics User Facility will enable researchers to perform high-throughput global ultrasensitive and quantitative proteomics measurements, and provide high-throughput identification and characterization of protein complexes, among other capabilities. The other centers will provide similar significant capabilities. In total, these systems biology research centers will operate on an integrated user facility basis and promote collaborative research to meet the demand for biological discovery in the 21 st century.
Multiprogram Research Building	We provide conferencing capability to support collaborations with other national laboratories, government agencies, academia, and industry. We provide a portal between scientific community and Laboratory user facility and laboratory capability. In partnership with academic institutions, we support the education and development of current and future scientists and engineers.
Engineering Research Laboratory	Expanded mission responsibilities are anticipated for DOE programs in fuel cell materials and technology, microtechnology, lightweight materials research for energy-efficient automobiles and trucks, advanced passive and active electronic sensors, advanced electronic systems, and bio-based processing. New facilities are needed for prototype testing and technology demonstration, materials synthesis, fabrication, storage, and computations. We anticipate the need for segregated work areas to accommodate the special confidentiality requirements of industrial partners.
Bio-Products Research Facility	Pacific Northwest National Laboratory involvement in agricultural and bio-products research since the mid-1970s has established the Laboratory as a leader in delivering science and technology solutions to the agriculture industry. The hallmark of our research is expertise in the area of novel chemical and biological processes for conversion of low-value or waste biomass to industrial and consumer products, fuels, and energy. These industrial and consumer products typically have a higher market value than biomass-derived fuel ethanol or energy, and the current worldwide marketplace is promising. By integrating state-of-the-art capabilities in chemistry, chemical engineering, and biology, we are establishing a host of new nonfood markets for agricultural products supporting the farming industry and reducing our reliance on foreign petroleum imports.
National Security Capability	We develop innovative solutions to critical national and international problems by applying and deploying the full science and technology capabilities of the Laboratory to our safety and security programs. The national security missions of the Laboratory will continue to expand. Proposed upgrades and modification to existing facilities may accommodate National Security 2010 capability requirements.

Table 6.3. Summary of Investments Needed to Support Laboratory Missions (contd)

Investment Area	Mission Support
Research Support Capability	Conferencing capability to support the collaborations with other national laboratories, government agencies, academia, and industry. Provides portal between scientific community and Laboratory user facility and laboratory capability. In partnership with academic institutions, supports of the education and development of current and future scientists and engineers.
EMSL II Capability	<p>EMSL Laboratory Upgrade–Phase 1</p> <p>The EMSL Laboratory Upgrade is the first of a three-phase project that will construct the physical structure to house the next generation EMSL research equipment and tools. These new, advanced capabilities will build upon the current six EMSL research capabilities to create new knowledge and deliver solutions to science and technology challenges across DOE science, national security, and environmental quality and energy resource missions. This project expands the laboratory capabilities of EMSL to accommodate the proposed 1.2 GHz NMR, the 21 Telsa FTICR Mass Spectrometer, a Catalysis & Exhaust Emission Science Facility, and expanded high resolution imaging capabilities described in the FY 2002 SC Onsite Review. The 1.2 GHz NMR will enable structural solutions to complex problems in biology, materials chemistry, and microimaging. The 21 Tesla FTICR mass spectrometer will enable proteomics studies of microbial communities. The catalysis and exhaust emission science facility will enable discoveries in catalysis and chemical transformation, providing new insights and technologies for emission control needed, for example, to meet challenging Diesel Emission Standards in 2007. Finally, expanded high resolution imaging capabilities are needed to achieve the goals of DOE's Genomes to Life program. This project takes advantage of the original EMSL design which provides the capability to add a laboratory pod on the north end of the building.</p>

descriptions and funding profiles (described in detail in the next section) balance high-priority environmental, safety, health, and infrastructure projects, and our science and technology needs. A portfolio management approach is used to maintain this balance among all of the Laboratory's needs. The fiscal year 2003-2013 needs funding chart illustrates current budgets and projected requirement in general purpose line-item construction, general plant project, general plant equipment, excess facilities and indirect real property maintenance.

Performance metrics being considered in support of infrastructure modernization focus on management of capital construction projects, condition of space and equipment, and actual maintenance as a percentage of replacement value.

6.5 Facility Modernization and Revitalization Resource Requirements

6.5.1 Modernization

Our Laboratory vision requires facilities to support advanced science and technology missions, new high-performance computers, specialized laboratory space for molecular and cellular biology, protected areas for national security missions,

Table 6.4. Modernization Is Driven by Mission Need			
	Space Added	Space Removed	TEC
Infrastructure Line Item Construction			
D-494, Systems Upgrade			9.9
EMSL Laboratory Upgrade–Phase 1	36,000 SF	0 SF	17.1
300 Area Replacement Facility–Phase 1	30,000 SF	30,000 SF	25.9
300 Area Replacement Utility Corridor			16.3
D-485, 320 Building Renovation			7.5
D-496, Laboratory Systems & Rehabilitation			9.7
Research Support Building	65,000 SF	0 SF	25.0
300 Area Replacement Facility–Phase 2	57,000 SF	57,000 SF	30.0
300 Area Replacement Facilities–Outyear	550,000 SF	663,000 SF	120.0
Engineering Research Laboratory	100,000 SF	0 SF	80.0
Total Line Items			341.9

process and engineering pilot-scale test research, and conferencing capability to enable research communication and collaboration. The current shortage of office space for Laboratory users complicates interim plans for creating this long-term vision. The sizing of new facilities and estimated costs are shown in Table 6.4 as ranges to reflect the current level of facility definition. The costs in the table are estimates for facility construction only and do not include estimates for design, management, or technical equipment.

6.5.2 Revitalization

The Laboratory capital facility revitalization projects are directed to the Science Laboratories Infrastructure Program and our two DOE Landlord offices. The priority system for capital facility requirements is risk-based to ensure that facilities and infrastructure are operated safely to protect our staff, the public, and the environment while addressing science and technology rehabilitation and infrastructure needs. The building life cycle plans and condition assessments are essential for identifying maintenance needs and for establishing facility priorities. Past maintenance investments have focused on updating the physical plant and other basic infrastructure revitalization issues. Because of this, future investment strategies mainly target options to address the research requirements of modern science.

Based on recent changes in DOE’s plans for the 300 Area cleanup a 300 Area exit strategy is under development with the objectives of retaining critical research capabilities, optimizing the useful life of the 300 Area buildings to support Hanford Accelerated Cleanup and risk reduction strategy, consolidating and modernizing the Laboratory facility footprint and building “clean to stay clean” thus creating no future DOE legacy.

Pacific Northwest National Laboratory will continue to look at ways for creative investment strategies to ensure good stewardship of DOE and Battelle capital resources to meet the most important DOE mission needs. Limited resources have motivated the Laboratory to pursue other funding mechanisms, such as Energy Saving Performance Contracts, to assist in reducing the backlog. Energy

Saving Performance Contracts is a creative investment strategy the Laboratory uses to provide resources for utility infrastructure improvements from the savings achieved by improved energy performance.

6.6 Science Laboratories Infrastructure – Facility Support Investments

We analyzed our critical Office of Science facilities to estimate the funding that would be needed to improve, refurbish or replace those facilities. Figure 6.4 and Table 6.5 highlight the total revitalization and modernization needs at the Laboratory. The investment will result in a significantly reduced deferred maintenance level due to the removal of the old, maintenance intensive facilities in the 300 Area. This plan is also responsive to all that is currently known about the 300 Area accelerated closure schedule.

6.6.1 FY 2002 Line Item – Laboratory Systems Upgrades (ongoing)

As the Plan for Restoration of the River Corridor moves forward, line item upgrades will be reviewed to ensure that upgrades are planned only for the buildings that will remain in place. This line item will upgrade the less-efficient building systems with retrofitted technology that increases the life span of the building while decreasing energy consumption and maintenance service costs. These systems include heating, ventilation, and air-conditioning components (replacement of supply and exhaust fans with both equipped with variable frequency drive systems). We will replace chemical exhaust fume hoods that cannot be retrofitted with variable air volume fans with controllable damper systems and modular controls for the vane dampening controls within the system. Heating and cooling systems in three buildings (329, 336, and 338) will be equipped with digital controls for existing supply and exhaust fans, inlet vanes, and isolation dampers.

Old, energy-inefficient chemical fume hoods will be replaced in two buildings (331 and 326). Ninety-seven hoods will be retrofitted or replaced to add variable air volume capability. This type of fume hood allows sashes to be closed when not in use. These controls will decrease operator service (manipulation time) and will allow control by computer-based systems. A natural-gas-powered electrical generator will be installed to decrease the cost of backup power at the 331 Building. Energy savings will be obtained by replacing failed glazing (cracked and broken single-pane glazing and double-glazing where the seals have failed) in the 326 and 337 buildings.

6.6.2 FY 2005 Line Item – EMSL Laboratory Upgrade – Phase I

The EMSL Laboratory Upgrade is the first of a three-phase project that will construct the physical structure to house the next generation EMSL research equipment and tools. These new, advanced capabilities will build upon the current six EMSL research capabilities to create new knowledge and deliver solutions to science and technology challenges across DOE science, national security, and environmental quality and energy resource missions. This project expands the

laboratory capabilities of EMSL to accommodate the proposed 1.2 GHz NMR, the 21 Tesla FTICR Mass Spectrometer, a Catalysis & Exhaust Emission Science Facility, and expanded high resolution imaging capabilities described in the Fiscal Year 2002 Office of Science Onsite Review. The 1.2 GHz NMR will enable structural solutions to complex problems in biology, materials chemistry, and microimaging. The 21 Tesla FTICR mass spectrometer will enable proteomics studies of microbial communities. The catalysis and exhaust emission science facility will enable discoveries in catalysis and chemical transformation, providing new insights and technologies for emission control needed, for example, to meet challenging Diesel Emission Standards in 2007. Finally, expanded high resolution imaging capabilities are needed to achieve the goals of DOE's Genomes to Life program. This project takes advantage of the original EMSL design which provides the capability to add a laboratory pod on the north end of the building.

Significant expansions to the Environmental Molecular Sciences Laboratory are planned in a phased approach, to help maximize the impact of this premier user facility.

6.6.3 FY 2006 Line Item-300 Area Multiprogramming Building Replacement-Phase I

PNNL's strategy of consolidating critical research capability out of weapon production and cold war aged buildings into a core set of PNNL facilities no longer appears viable. There is an immediate need to relocate critical research activities out of, and close to, PNNL buildings which are at the end of their mission or functional life. This project constructs a 43,000 gross square foot replacement facility near EMSL. The multiprogram facility is configured of ~25,000 square foot laboratory, ~10,000 square foot office, and ~4,000 square foot storage space. This project is the first step in making 750,000 gross square feet of old and contaminated buildings, and associated legacy waste available for Office of Environmental Management funded disposition.

6.6.4 FY 2006 Line Item-300 Area Utility Distribution System Replacement

The Office of Environmental Management currently is responsible for delivering site and utility services to Pacific Northwest National Laboratory buildings located on the Hanford site. The 300 Area utility distribution system supports many Pacific Northwest National Laboratory occupied government owned buildings. Large-scale Office of Environmental Management cleanup of the 300 Area will require extensive excavation and will result in severance of water, sewer and electrical distribution systems. Reconfiguration and replacement of these systems will be required.

6.6.5 FY 2006 Line Item-320 Building Infrastructure Rehabilitation (alternative)

The 320 Building is recognized as one of our core DOE facilities. The 320 Building was built in 1964, and because of age and heavy use, it is deteriorating. We requested funding from the Office of Science in 1999 to rehabilitate the 320 Building to decrease operating and maintenance costs and to provide a safer and more productive work environment. This project will upgrade this strategic laboratory and its facility systems to extend its useful lifetime. Existing systems, including the heating, ventilation, and air-conditioning systems, will be modernized with highly efficient equipment and controls to reduce energy and operational costs.

Existing conditions in the facility result in a waste of 5 percent to 10 percent of research staff hours annually (or \$300,000 to \$600,000). These system modifications will eliminate excessive vibration caused by heating, ventilation, and air-conditioning equipment that interferes with performance of sensitive microscopes and spectrometers. These upgrades will be required if the 300 Area accelerated cleanup relocation plan is not supported or the cleanup schedule is extended.

6.6.6 FY 2006 Line Item–Laboratory Systems and Rehabilitation Upgrade (alternative)

This project is part of the continued revitalization efforts ongoing at the Laboratory over the last 10 years. The revitalization efforts over the past decade focused on the physical plant in the strategic facilities in the 300 Area. This project supports the continuing revitalization plan and initiates the next decade of revitalization focused at laboratory and administrative space upgrades. The activities performed as a result of this project will help ensure that these laboratories effectively support the research and development programs being accomplished in these facilities. Planned upgrades are estimated to reduce utility and operation and maintenance costs. Optimizing research and administrative office use will increase space utilization efficiency. Operating cost savings will result primarily from converting to variable air volume heating, ventilating, and air-conditioning systems in 329 Building laboratories. Needed research office space will be provided by addition of an office wing on the 331 Building, and space use will be improved by renovation of open bay office areas in the 337 Building. These upgrades will be required if the PNNL 300 Area accelerated cleanup relocation plan is not supported or the cleanup schedule is extended.

6.6.7 FY 2007 –Research Support Capability

The Research Support Capability will be an approximately 50,000 gross square feet facility to house conferencing capability, lecture halls, science and technology demonstration space, seminar rooms, and leading edge information technology and communication systems. The facility will create the entrance point to the Laboratory campus and the gateway for visitors and collaborators to again access to Laboratory capabilities-staff, facilities, and equipment. It will be the center for meetings, collaborations, and for exchanging scientific ideas. It will also house on-site food services.

6.6.8 FY 2007 Line Item–300 Area Multiprogramming Building Replacement–Phase 2

This is the second in a series of replacement buildings that will house critical research capabilities relocated from the 300 Area clean-up zone to a central campus next to EMSL. This project will allow the Office of Environmental Management funded disposition of part of the 750,000 gross square feet of facilities that Pacific Northwest National Laboratory occupies in the 300 Area while maintaining critical research capabilities and programs. The project includes construction of a 57,000 gross-square-foot facility to replace laboratory, office, and storage capability consolidated from Pacific Northwest National Laboratory 300 Area buildings.

6.6.9 General Plant Equipment

Pacific Northwest National Laboratory has an equipment plan to support the Laboratory mission over the next 5 years. This plan requires an annual investment of \$2 million.

6.7 Identifying and Prioritizing Infrastructure Modernization Projects

At Pacific Northwest National Laboratory, each research directorate seeks input on needed human, equipment, and facility resources from multiple sources, including research staff, customers, university research partners and collaborators, end users, and user advisory committees. The formality of obtaining and documenting input from various external sources depends on the nature and maturity of the relationship itself and ranges from one-on-one meetings to workshops to formal project reviews. In the latter category, the Environmental Molecular Sciences Laboratory's User Advisory Committee reviews user feedback and equipment utilization data to provide recommendations on equipment and facility acquisitions and modifications. These recommendations are submitted for consideration through the Laboratory's annual business planning process.

The Laboratory's research directorate review committees, which are composed of representatives from government, academia, and industry from around the nation, meet annually to review their respective directorate's business (strategic) plan, the quality and relevance of research performed, and evaluate the effectiveness of technical capability stewardship. Facility and equipment capability, though a small part of the review, is a part of the technical capability discussion. Recommendations for facility and equipment capability development resulting from the research directorate review committees are included in each directorate's annual business plan.

Pacific Northwest National Laboratory also seeks input on infrastructure needs from Laboratory researchers who are defined as the lead in evaluating the appropriateness of a project's technical scope, schedule, and cost. As such, members of the Laboratory research community join with the facility planning staff to integrate and prioritize submitted requirements and develop, under the leadership of the Laboratory's Facility Management System in the Facilities and Operations Directorate, the 10-year facilities strategic plan.

The Laboratory's Management Council reviews and approves the 10-year facility strategic plan and each directorate's annual business plan as part of the investment decision process. The 10-year facility strategic plan in its entirety is not formally reviewed with external stakeholders, other than DOE. Research directorates share information of specific interest with clients and stakeholders through the same means used to gather new requirements.

Pacific Northwest National Laboratory's process is effective and has led to the construction of needed capability identified by Laboratory users and collaborators, including the Applied Process Engineering Laboratory, sited at the Port of Benton. It has also, and in concert with a recent Office of Biological and Environmental Research Advisory Committee review, identified the need for new biological and computational sciences facilities for which Pacific Northwest National Laboratory



Figure 6.4. PNNL Infrastructure Modernization and Revitalization Needs Chart

plans to compete. Pacific Northwest National Laboratory is now teaming with Washington State University to construct a bio-products research laboratory on the university’s campus to serve the needs of the university community and DOE.

6.8 Assets Management

Pacific Northwest National Laboratory’s intent is to maintain facilities and equipment in a manner that will allow the full benefit of the design life. The criteria for which organizations can return space within a facility are established to address legacy issues (materials, chemicals, equipment). The vacating organization is allowed to leave the space without removing equipment and material or restoring the space to its original configuration only if another organization is willing to accept the space in its existing condition and any associated legacy issues. When a facility or equipment no longer meets a program’s needs, an assessment is made to determine whether replacement is needed and if the existing asset can be converted economically into an alternative use. If divesting and disposition of an existing facility is prudent, the facility is put in a condition that will ensure the health and well-being of the workers, the public, and the environment.

6.9 Energy Management

In the last 12 months, Pacific Northwest National Laboratory has implemented building and grounds recommissioning campaigns that have annually avoided

Table 6.5. Needs Summary Table to Support Modernization Needs Funding Chart

	Space Added+	Space Removed+	TEC	Modernization Needs											
				2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
Indirect Funded Maintenance (DOE Facilities) ^(a)				4.03	3.70	3.81	5.10	5.26	5.41	5.58	5.74	5.92	6.09	6.28	6.46
(% of RPV)				1.16%	1.16%	1.16%	1.16%	1.16%	1.16%	1.16%	1.16%	1.16%	1.16%	1.16%	1.16%
Indirect Funded Maintenance (BMI Facilities) ^(a)				2.93	2.97	3.06	3.03	3.13	3.29	3.32	3.41	3.52	3.62	3.73	3.85
Total Indirect Maintenance				6.96	6.68	6.88	8.14	8.40	8.71	8.91	9.16	9.45	9.72	10.02	10.32
Estimated Deferred Maintenance-SC				46.12	60.83	73.68	87.88	94.03	98.89	104.08	89.26	92.25	95.26	96.73	97.85
Estimated Deferred Maintenance-EM				21.80	25.28	30.19	37.05	33.42	37.83	39.32	40.06	40.54	40.51	44.24	45.50
Total Deferred Maintenance				67.92	86.21	103.87	124.93	127.45	136.72	143.40	129.32	132.79	135.77	140.97	143.35
Investments Reducing Deferred Maintenance															
Line Items				9.90		1.17	6.73	1.00	6.70	27.00					111.10
GPP				3.94	3.94	3.50	9.50	5.00	4.50	4.50	8.30	8.50	5.60	5.80	6.00
IGPP					1.00	3.50									
Indirect Funded Maintenance				0.40	0.37	0.38	0.51	0.53	0.54	0.56	0.57	0.59	0.61	0.63	0.65
Total Reductions				14.24	5.31	8.55	16.74	6.53	11.74	32.06	8.87	9.09	6.21	6.43	117.75
Net Deferred Maintenance				53.68	80.90	95.32	108.19	120.92	124.98	111.34	120.45	123.70	129.56	134.54	25.60
GPP: DOE – SC ^(b)															
D-493, 326 “B” Floor – Laboratory Upgrades (contd)			0.77	1.12											
D-498, 326 “A” Floor – Laboratory Upgrades			2.81	0.58	2.23	0.00									
D-497, 331 3rd Floor South – Lab Upgrades			0.82	0.82											
D-499, 331 3rd Floor Center – Lab Upgrades			0.99	0.34	0.65										
D-500, 3rd Floor North & 1st Floor Lab Upgrades			2.50	0.10	2.05	0.08									
329 “C” Section Modifications			2.00		0.20	1.80									
EMSL Office Addition			4.70			0.20	2.50	2.00							
331A Aquatics Lab Expansion			1.50		0.50	0.50	0.50								
337 seal roof of main mechanical room and hotwater conversion			0.41			0.41									
350 Roof Replacement/Changeroom Mods/Convert to Natural Gas			0.50			0.50									
EMSL Shop Modifications			0.25		0.25										
Infrastructure Revitalization			1.00				0.50	0.50							
Other			40.30	0.56			0.50	1.50	5.00	5.10	5.30	5.50	5.60	5.80	6.00
Total SC GPP			58.55	3.52	5.88	3.49	4.00	4.00	5.00	5.10	5.30	5.50	5.60	5.80	6.00

Table 6.5. Needs Summary Table to Support Modernization Needs Funding Chart (contd)

	Space Added+	Space Removed+	TEC	Modernization Needs											
				2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
GPP: DOE – EM ^(c)															
325 Renovation Upgrades				0.00	0.00	0.00	8.50	3.00	3.00	3.00	3.00	3.00			
Total SC & EM GPP			82.69	3.52	5.88	3.49	12.50	7.00	8.00	8.10	8.30	8.50	5.60	5.80	6.00
GPE															
Information Technology				0.80	0.81	1.86	1.80	1.90	2.00	2.00	2.00	2.10	2.10	2.20	2.30
Other GPE Priorities				0.27	0.19	0.39	0.39	0.40	0.41	0.43	0.44	0.45	0.47	0.48	0.49
Total GPE			26.67	1.07	1.00	2.25	2.19	2.30	2.41	2.43	2.44	2.55	2.57	2.68	2.79
Infrastructure Line Item Construction															
D-494, Systems Upgrade			9.90	9.90											
EMSL Laboratory Upgrade-Phase 1	36,000 SF		15.90				15.90								
300 Area Replacement Facility-Phase 1	30,000 SF		26.00					26.00							
300 Area Replacement Utility Corridor			16.30					16.30							
D-485, 320 Building Renovation			7.50												
D-496, Laboratory Systems & Rehabilitation Upgrades			9.70												
Research Support Building	65,000 SF		25.00						25.00						
300 Area Replacement Facility- Phase 2	170,000 SF		30.00						30.00						
300 Area Replacement Facilities- Outyear			120.00							30.00	30.00	30.00	30.00		
Engineering Research Laboratory	100,000 SF		80.00							80.00					
Line Item Construction (Programmatic)															
Systems Biology Capability (Genomes to Life) ^(d)	Up to 140,000 SF		Up to 175.00				175.00								
Total Line Items			340.30	9.90	0.00	0.00	190.90	42.30	55.00	110.00	30.00	30.00	30.00	0.00	0.00
Total GPP/GPE/Line Items			425.52	14.49	6.88	5.73	205.59	51.60	65.41	120.53	40.74	41.05	38.17	8.48	8.79
Excess Facilities Clean-up and Disposition^(e)															
3720, 306-W, 323, 3730, 3718-P, 305-B		94,524 SF													
Administrative			1.72	0.01	0.01	0.01	0.39	0.03	0.76	0.27	0.18	0.02	0.02	0.01	0.01
Project D&D			41.86	0.00								41.86			
Total			43.58	0.01	0.01	0.01	0.39	0.03	0.76	0.27	0.18	41.88	0.02	0.01	0.01
Spaced Disposition 1995-2001															
DOE		389,365 SF													
Battelle Northwest		43,331 SF													

Table 6.5. Needs Summary Table to Support Modernization Needs Funding Chart (contd)

	Space Added+	Space Removed+	TEC	Modernization Needs											
				2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
Third Party Funding															
Computational & Analytical Sciences Building	100,000 SF		30.00			30.00									
Bio-Ag Building	60,000 SF		23.00						23.00						
BMI Capital Needs at Pacific Northwest^(f)															
Annex			1.20	0.00	0.06	0.25	0.50	0.08	0.00	0.00	0.00	0.00	0.10	0.21	
Auditorium			1.34	0.50	0.54	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.15	0.10	
BRSW			0.56	0.00	0.08	0.05	0.00	0.36	0.00	0.00	0.00	0.04	0.00	0.03	
CEL			0.93	0.00	0.00	0.30	0.53	0.03	0.00	0.00	0.00	0.01	0.01	0.05	
EDL			0.45	0.00	0.10	0.05	0.03	0.02	0.06	0.15	0.04	0.00	0.00	0.00	
ESB			0.33	0.00	0.00	0.05	0.03	0.00	0.03	0.13	0.00	0.03	0.04	0.02	
Leased Buildings			0.45	0.10	0.05	0.00	0.00	0.00	0.05	0.05	0.05	0.05	0.05	0.05	
LSL-II			3.84	1.25	0.37	0.67	0.30	0.90	0.34	0.32	0.25	0.11	0.00	0.00	
Math			0.60	0.08	0.10	0.10	0.06	0.10	0.00	0.03	0.03	0.05	0.05	0.00	
MSL-1			0.23	0.00	0.15	0.00	0.04	0.00	0.04	0.00	0.00	0.00	0.00	0.00	
MSL-2			0.20	0.00	0.07	0.00	0.02	0.00	0.00	0.01	0.01	0.00	0.02	0.07	
MSL-3			0.18	0.00	0.08	0.00	0.03	0.01	0.00	0.00	0.03	0.00	0.03	0.00	
MSL-5			1.05	0.25	0.14	0.11	0.30	0.06	0.08	0.00	0.03	0.01	0.07	0.00	
PDLE			0.67	0.00	0.05	0.20	0.08	0.00	0.02	0.00	0.00	0.00	0.22	0.10	
PDLW			0.92	0.00	0.03	0.30	0.13	0.03	0.30	0.02	0.04	0.04	0.03	0.00	
PSL			4.43	0.20	0.13	1.13	0.08	0.03	0.00	0.36	0.75	1.03	0.50	0.22	
ROB			1.81	0.00	0.52	0.30	0.10	0.10	0.10	0.28	0.13	0.00	0.08	0.20	
RRC			27.66	2.95	2.20	2.61	3.50	2.10	2.90	2.70	2.40	2.40	2.25	1.65	
RTL			3.11	0.40	0.43	0.32	0.38	0.80	0.20	0.12	0.10	0.08	0.13	0.15	
Total BMI Capital			49.96	5.73	5.10	5.82	6.11	4.62	4.12	4.17	3.86	3.85	3.73	2.85	0.00
Total Third Party			102.96	5.73	5.10	35.82	6.11	4.62	27.12	4.17	3.86	3.85	3.73	2.85	0.00

(a) Indirect funded Real Property Maintenance.

(b) GPP beyond 2007 is based on past planned work plus escalation. Specific projects will be defined at a later date.

(c) Outyear EM GPP (FY 2006 and beyond) requirements represent an estimated steady state of investment to maintain operational condition of facility.

(d) Line item total does not include programmatic funded Genomes to Life.

(e) Includes planned 300 Area accelerated cleanup facilities D&D cost.

(f) Figures derived from Facility Condition Assessments.

SF = square feet.

220 million gallons of Columbia River water (a key ecological resource for the Pacific Northwest), and over \$250,000 in energy cost. The Laboratory facility management staff partnered with research staff to develop, test, and apply software for automatic and continuous measurement and verification of building performance. Early efforts at recommissioning served as a springboard for many of the Federal Energy Management Program's ALERT program concepts, which were applied across federal facilities nationwide. The Laboratory facility management leveraged its relationships with research to seek and receive Federal Energy Management Program funding to improve infrastructure and implement sustainable concepts in the facility design processes. In October 2001, Pacific Northwest National Laboratory received over \$227,000 in federal funding for this purpose. These successes have resulted in invitations to present at Energy 2002, industry forums, and Energy Cross-Talk 2002, a peer-to-peer exchange between energy professionals from industry and government. During 2002, Pacific Northwest National Laboratory is seeking ENERGY STAR status for the Sigma 5 building and incorporating Leadership Energy and Environmental Design criteria in the request for proposal for a planned office/laboratory building. Two facility engineering staff have completed their Leadership Energy and Environmental Design certification.

Through collaboration with pollution prevention staff and the City of Santa Monica, Laboratory facility management staff were able to replace its hazardous cleaning agents with bio-based and green cleaners that keep workers' health and the environment as clean as the windows and walls. Instead of using more than 30 cleaning products, custodians now use 7, one of which is the key product in the suite, the bio-based cleaner. The Laboratory is now sharing its experience with a local school district that hopes to benefit by providing a healthier environment for school children.

Our Facility Transition program has created the procedures and systems needed to identify appropriate surveillance and maintenance activities and opportunities to excess unneeded property in a cost-effective manner.

Resource Projections

The resource requirements of research and development for Hanford Site support are included in the resource projections of the various funding programs. Research and development for other U.S. Department of Energy sites at other DOE facilities, however, are shown as a separate program. The resource projections for fiscal years 2001 and 2002 are actual values.

Table 7.1. Laboratory Funding Summary

(Budget Authorization Dollar Amount in Millions)

	2001	2002	2003	Fiscal Year			
				2004	2005	2006	2007
DOE Effort	420.9	441.4	428.2	430.1	446.4	464.6	473.1
Work for Others	41.0	75.7	92.5	91.4	91.7	97.4	102.7
Total Operating	461.9	517.1	520.7	521.5	538.1	562.0	575.7
Capital Equipment	14.0	9.1	5.9	8.8	9.1	11.4	11.7
General Purpose Equipment-GPE	--	--	4.0	4.0	4.0	4.0	4.0
General Plant Projects-GPP	6.2	4.8	4.0	4.0	4.0	4.0	4.0
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Gross Laboratory Funding	482.1	531.0	535.6	539.3	579.5	596.3	599.4
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Net Laboratory Funding	425.8	468.1	479.5	480.1	519.3	534.1	535.3

Table 7.2. Laboratory Personnel Summary

(Full-Time Equivalent [FTEs])

	2001	2002	2003	Fiscal Year			
				2004	2005	2006	2007
DOE Effort	1,233	1,190	1,194	1,226	1,251	1,283	1,326
Work for Others	159	211	212	217	223	228	235
Total Operating	1,392	1,401	1,406	1,443	1,474	1,511	1,560
Capital Equipment	3	4	4	4	4	4	4
General Purpose Equipment-GPE							
General Plant Projects-GPP	10	6	4	4	4	4	4
Construction Line Items	--	--	4	4	19	14	4
Total Direct	1,405	1,411	1,417	1,454	1,490	1,529	1,572
Indirect	1,381	1,423	1,441	1,458	1,485	1,507	1,526
Total Laboratory Personnel (FTE)	2,786	2,834	2,858	2,912	2,975	3,036	3,098

Table 7.3. Funding by Secretarial Officer

(Budget Authorization Dollar Amount in Millions)

	2001	2002	2003	Fiscal Year			2007
				2004	2005	2006	
Office of Science							
Operating	50.6	54.8	69.2	77.4	87.6	93.7	98.1
EMSL Operations - Expense	26.7	33.8	36.0	39.5	41.9	44.4	47.0
Capital Equipment	6.9	3.4	3.9	4.3	4.3	6.3	6.3
EMSL Operations Capital Equipment	4.4	3.8	2.0	4.5	4.8	5.1	5.4
General Purpose Equipment-GPE	--	--	1.0	1.0	1.0	1.0	1.0
General Plant Projects-GPP	4.0	4.8	4.0	4.0	4.0	4.0	4.0
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Total	92.5	100.6	117.1	131.7	167.9	169.4	165.8
Office of Environmental Restoration and Waste Management							
Operating	99.4	111.7	99.3	103.6	106.9	110.2	112.5
Capital Equipment	0.1	0.5	--	--	--	--	--
General Purpose Equipment-GPE	--	--	3.0	3.0	3.0	3.0	3.0
General Plant Projects-GPP	2.2	--	--	--	--	--	--
Construction Line Item	--	--	--	--	--	--	--
Total	101.7	112.2	102.3	106.6	109.9	113.2	115.5
Assistant Secretary for Energy Efficiency and Renewable Energy							
Operating	27.6	26.9	30.6	34.1	38.1	41.6	45.5
Capital Equipment	0.1	--	--	--	--	--	--
Total	27.7	26.9	30.6	34.1	38.1	41.6	45.5
Assistant Secretary for Environment, Safety and Health							
Total Operating	1.9	0.4	0.7	0.9	0.9	0.9	0.9
National Nuclear Security Administration (NNSA)							
Assistant Secretary for Defense Programs							
Operating	41.5	23.1	9.0	5.9	7.5	7.9	8.0
Capital Equipment	1.3	--	--	--	--	--	--
Subtotal Defense Programs	42.8	23.1	9.0	5.9	7.5	7.9	8.0
Office of Defense Nuclear Nonproliferation							
Operating	113.5	140.4	137.7	118.7	110.3	112.2	105.9
Capital Equipment	0.4	1.1	--	--	--	--	--
Construction Line Items	--	--	--	--	--	--	--
Subtotal Defense Nuclear Nonproliferation	113.9	141.5	137.7	118.7	110.3	112.2	105.9
Operating	155.0	163.5	146.7	124.6	117.8	120.1	113.9
Capital Equipment	1.7	1.1	--	--	--	--	--
Construction Line Items	--	--	--	--	--	--	--
Total National Nuclear Security Administration	156.7	164.6	146.7	124.6	117.8	120.1	113.9

Table 7.3. Funding by Secretarial Officer (contd)

(Budget Authorization Dollar Amount in Millions)

	2001	2002	2003	Fiscal Year 2004	2005	2006	2007
Office of Energy Assurance							
Total Operating	--	0.6	0.6	0.6	0.6	0.6	0.6
Office of Intelligence							
Total Operating	5.9	4.9	4.0	4.1	4.3	4.5	4.6
Office of Counterintelligence							
Total Operating	13.2	14.3	13.3	13.5	14.0	14.3	14.5
Capital Equipment	--	--	--	--	--	--	--
Total	13.2	14.3	13.3	13.5	14.0	14.3	14.5
Assistant Secretary for Nuclear Energy							
Total Operating	1.3	0.8	3.1	4.4	3.9	5.6	5.6
Office of Security and Emergency Operations							
Total Operating	16.2	5.4	3.6	3.6	3.6	3.3	3.2
Capital Equipment	0.5	--	--	--	--	--	--
Total	16.8	5.4	3.6	3.6	3.6	3.3	3.2
Assistant Secretary for Fossil Energy							
Total Operating	5.3	7.1	7.1	8.4	10.8	11.6	12.4
Capital Equipment	0.3	0.3	--	--	--	--	--
Total	5.6	7.4	7.1	8.4	10.8	11.6	12.4
Office of Policy, Planning and Program Evaluation							
Total Operating	--	--	--	--	--	--	--
Other DOE Organizations							
Operating	0.5	1.1	2.6	3.8	4.3	1.8	1.8
General Plant Projects-GPP	--	(0.0)	--	--	--	--	--
Total	0.5	1.1	2.6	3.8	4.3	1.8	1.8
Other DOE Sites							
Operating	17.4	16.2	11.6	11.7	11.8	12.2	12.6
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Total DOE Sites	(38.9)	(46.8)	(44.4)	(47.4)	(48.4)	(50.0)	(51.6)
Total DOE Programs							
Operating	420.9	441.4	428.2	430.1	446.4	464.6	473.1
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Capital Equipment	14.0	9.1	5.9	8.8	9.1	11.4	11.7
General Purpose Equipment-GPE	--	--	4.0	4.0	4.0	4.0	4.0
General Plant Projects-GPP	6.2	4.8	4.0	4.0	4.0	4.0	4.0
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Total	384.8	392.4	387.1	388.8	427.6	436.7	432.6

Table 7.3. Funding by Secretarial Officer (contd)

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Work for Others							
Department of Defense	25.7	42.0	50.8	52.2	54.8	57.2	59.1
Nuclear Regulatory Commission	4.3	5.8	6.8	7.0	7.4	7.6	7.8
Environmental Protection Agency	1.0	2.2	4.0	4.4	4.8	5.3	5.9
Dept. of Health and Human Svcs./NIH	0.3	0.1	2.0	3.5	5.0	6.5	8.0
NASA	0.1	0.2	0.8	0.8	0.8	0.8	0.8
U.S. Customs	0.5	11.7	10.0	5.6	--	--	--
IRS	3.9	0.3	4.0	4.0	4.0	4.0	4.0
Department of State	0.4	4.1	0.7	--	--	--	--
Other Federal Agencies	2.8	7.1	7.6	8.1	8.5	9.0	9.4
Other - Non-Federal Agencies	2.1	2.3	5.9	5.9	6.4	7.0	7.7
Total	41.0	75.7	92.5	91.4	91.7	97.4	102.7
Total Laboratory Funding							
Operating	461.9	517.1	541.9	517.1	539.3	563.2	577.0
Capital Equipment	14.0	9.1	5.9	8.8	9.1	11.4	11.7
General Purpose Equipment-GPE	--	--	4.0	4.0	4.0	4.0	4.0
General Plant Projects-GPP	6.2	4.8	4.0	4.0	4.0	4.0	4.0
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Gross Laboratory Funding	482.1	531.0	535.6	539.3	579.5	596.3	599.4
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Net Laboratory Funding	425.8	468.1	479.5	480.1	519.3	534.1	535.3

Table 7.4. Direct Personnel by Secretarial Officer

(Personnel in FTE)

	2001	2002	2003	Fiscal Year 2004	2005	2006	2007
Office of Science							
Operating	232	268	282	299	297	310	328
Office of Environmental Restoration and Waste Management							
Operating	407	413	408	412	416	425	430
Assistant Secretary for Energy Efficiency and Renewable Energy							
Operating	97	95	95	98	100	103	106
Assistant Secretary for Environment, Safety and Health							
Operating	8	5	6	6	6	6	6
National Nuclear Security Adminis- tration (NNSA) Deputy Administrator for Defense Programs							
Operating	130	64	64	66	67	69	71
Deputy Administrator for Defense Nuclear Nonproliferation							
Operating	180	183	177	180	194	194	204
Total National Nuclear Security Administration (NNSA)							
Operating	310	247	241	246	261	263	275
Office of Energy Assurance							
Operating	--	1	1	1	1	1	1
Office of Intelligence							
Operating	26	20	20	21	21	22	22
Office of Counterintelligence							
Operating	48	49	50	51	52	54	55
Assistant Secretary for Nuclear Energy							
Operating	5	2	2	3	3	3	3
Office of Security and Emergency Operations							
Operating	20	19	19	19	20	20	21
Assistant Secretary for Fossil Energy							
Operating	18	16	16	17	17	18	18
Office of Policy, Planning and Program Evaluation							
Operating	--	--	--	--	--	--	--

Table 7.4. Direct Personnel by Secretarial Officer (contd)

(Personnel in FTE)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Other DOE Organizations							
Operating	2	6	6	6	6	6	6
Other DOE Sites							
Operating	60	49	49	50	51	53	54
Total DOE Programs (Operating)	1,232	1,190	1,195	1,227	1,257	1,288	1,326
Work for Others							
Department of Defense	87	127	96	129	137	139	142
Nuclear Regulatory Commission	16	19	13	15	19	19	19
Environmental Protection Agency	4	6	8	11	12	13	14
Dept. of Health and Human Svcs./NIH	1	0	13	18	22	24	26
NASA	0	1	1	2	2	2	2
U.S. Customs	2	34	57	16	--	--	--
IRS	12	1	8	8	10	10	10
Department of State	0	8	1	--	--	--	--
Other Federal Agencies	28	11	3	5	5	5	6
Other - Non-Federal Agencies	8	2	11	13	17	17	17
Total	159	211	212	217	223	228	235
Laboratory Direct							
Operating	1,392	1,401	1,406	1,443	1,479	1,516	1,560
Capital Equipment	3	4	4	4	4	4	4
General Plant Projects-GPP	10	6	4	4	4	4	4
Construction Line Items	--	--	4	4	19	14	4
Total Laboratory Direct	1,405	1,411	1,417	1,455	1,505	1,538	1,572
Total Laboratory Indirect	1,381	1,423	1,441	1,458	1,485	1,507	1,526
Total Laboratory Personnel (FTE)	2,786	2,834	2,858	2,913	2,990	3,045	3,098

Table 7.5. Resources by Major DOE Areas

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Office of Science							
Magnetic Fusion (AT)	1.3	1.4	1.4	1.4	1.4	1.4	1.4
Basic Energy Sciences (KC)	12.2	12.2	12.5	13.8	14.6	14.7	14.9
ER Scientific Computing Research (KJ)	4.3	4.1	6.1	7.5	6.9	7.8	8.6
Energy Research Analysis (KD)	0.4	0.4	0.4	0.4	0.4	0.4	0.4
Biological and Environmental Research (KP)	32.0	35.6	47.8	53.3	63.3	68.4	71.8
EMSL Operations - Expense (KP-BER)	26.7	33.8	36.0	39.5	41.9	44.4	47.0
Office of Science Pro. Dir. (KX, Univ Sci Ed)	0.3	0.6	1.0	1.0	1.0	1.0	1.0
Other (KA, KB, KH)	--	0.6	--	--	--	--	--
Total Operating	77.3	88.6	105.2	116.9	129.5	138.1	145.1
Capital Equipment (AT)	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Capital Equipment (KC)	0.8	1.1	1.2	1.2	1.2	1.2	1.2
Capital Equipment (KJ)	0.4	0.0	--	--	--	--	--
Capital Equipment (KP)	5.6	2.2	2.6	3.0	3.0	5.0	5.0
EMSL Operations Capital (KP-BER)	4.4	3.8	2.0	4.5	4.8	5.1	5.4
Capital Equipment	11.3	7.2	5.9	8.8	9.1	11.4	11.7
General Purpose Equipment-GPE (KP)	--	--	1.0	1.0	1.0	1.0	1.0
General Plant Projects-GPP (KP)	4.0	4.8	4.0	4.0	4.0	4.0	4.0
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Total Funding	92.5	100.6	117.1	131.7	167.9	169.4	165.8
Direct Personnel							
Operating	232	268	277	295	299	316	328
Capital	3	4	4	4	4	4	4
General Plant Projects-GPP	1	6	4	4	4	4	4
Construction Line Items	--	--	4	4	19	14	4
Total Direct Personnel	235	278	288	306	325	338	340
Office of Environmental Restoration and Waste Management							
Technology Development (EW)	21.1	20.1	0	0	0	0	0
Waste Management (EW)	58.8	39.7	54.0	57.0	59.0	60.0	61.0
Waste Management (EX)	--	--	--	--	--	--	--
Environmental Restoration (EW)	19.4	43.5	35.9	37.0	38.0	40.0	41.0
Environmental Restoration (EX)	--	--	--	--	--	--	--
Safeguards and Security (FS30)	--	8.4	9.4	9.6	9.9	10.2	10.5
Total Operating	99.4	111.7	99.3	103.6	106.9	110.2	112.5
Capital Equipment (EW/EX)	0.1	0.5	--	--	--	--	--
General Purpose Equipment-GPE	--	--	3.0	3.0	3.0	3.0	3.0
General Plant Projects-GPP	2.2	--	--	--	--	--	--
Construction Line Items	--	--	--	--	--	--	--
Total Funding	101.7	112.2	102.3	106.6	109.9	113.2	115.5
Direct Personnel							
Operating	407	413	413	415	419	425	430
Capital Equipment	0	0	0	--	--	--	--
General Plant Projects-GPP	9	--	--	--	--	--	--
Construction Line Items	--	--	--	--	--	--	--
Total Direct Personnel	416	413	413	415	419	425	430

Table 7.5. Resources by Major DOE Areas (contd)

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Assistant Secretary for Energy							
Efficiency and Renewable Energy							
Solar Energy (EB)	1.6	3.5	3.0	3.5	4.0	4.5	5.0
Buildings Sector-(EC)	10.0	8.6	7.5	7.5	8.0	8.0	9.0
Industrial Energy Conservation (ED)	3.0	2.2	7.6	9.6	11.5	13.8	15.5
Transportation Sector (EE)	9.0	8.2	10.0	11.0	11.6	12.3	13.0
Tech. and Financial Assistance (EF)	--	--	--	--	--	--	--
In-House Energy Management (WB)	0.2	--	--	--	--	--	--
Policy and Management (EH)	0.3	0.2	--	--	--	--	--
Federal Emergency Mgmt. (EL)	3.4	2.6	2.5	2.5	3.0	3.0	3.0
Power Technologies (EO)	--	1.5	--	--	--	--	--
Operating	27.6	26.9	30.6	34.1	38.1	41.6	45.5
Capital Equipment (ED)	0.1	--	--	--	--	--	--
Total Funding	27.7	26.9	30.6	34.1	38.1	41.6	45.5
Direct Operating Personnel	97	95	95	98	100	103	106
Assistant Secretary for Environment, Safety and Health							
Environmental, Safety and Health (HA-01)	0.2	0.2	--	--	--	--	--
Envir. Safety and Health-Non Def. (HC)	1.2	0.1	0.6	0.8	0.8	0.8	0.8
Envir. Safety and Health-Defense (HD)	0.5	0.1	0.1	0.2	0.2	0.2	0.2
Total Funding	1.9	0.4	0.7	0.9	0.9	0.9	0.9
Direct Operating Personnel	8	5	6	6	6	6	6
National Nuclear Security Administration (NNSA)							
Deputy Administrator for Defense Programs							
Weapons Activities (DP Operating)	41.5	21.8	8.0	4.9	6.3	6.7	6.8
DP Capital Equipment	1.3	--	--	--	--	--	--
Safeguards and Security (FS20 Operating)	--	1.3	1.0	1.0	1.2	1.2	1.2
FS Capital Equipment	--	--	--	--	--	--	--
Operating	41.5	23.1	9.0	5.9	7.5	7.9	8.0
Capital Equipment	1.3	--	--	--	--	--	--
Direct Operating Personnel	130	64	64	66	67	69	71
Naval Reactors							
AJ Operating	--	--	--	--	--	--	--
AJ Capital Equipment	--	--	--	--	--	--	--
Direct Personnel							
Operating	--	--	--	--	--	--	--
Capital Equipment	--	--	--	--	--	--	--
Total Direct Personnel	--	--	--	--	--	--	--

Table 7.5. Resources by Major DOE Areas (contd)

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Deputy Administrator for Defense							
Nuclear Nonproliferation							
Verification and Control Technology (NA-22)	18.1	20.5	19.0	20.0	23.0	25.0	27.0
International Nuclear Safety and Cooperation (NA-23)	65.7	52.9	60.8	44.4	36.8	35.0	30.0
Arms Control and Nonproliferation (NA-24)	9.8	14.1	9.6	9.8	10.0	10.2	10.4
International Material Protection and Emergency (NA-25)	15.5	50.2	45.0	40.0	35.0	35.0	30.0
U.S. Surplus Fissile Materials Disposition (NA-26)	4.3	2.6	3.3	4.5	5.5	7.0	8.5
Operating	113.5	140.4	137.7	118.7	110.3	112.2	105.9
Capital Equipment (NA-22)	0.4	1.1	--	--	--	--	--
Capital Equipment (NA-24)	--	--	--	--	--	--	--
Capital Equipment (NA-25)	--	--	--	--	--	--	--
Capital Equipment (NA-26)	--	--	--	--	--	--	--
Capital Equipment	0.4	1.1	--	--	--	--	--
Operating Personnel	180	183	177	180	194	194	204
Capital Equipment Personnel	0	0	--	--	--	--	0
Total Direct Personnel	180	183	177	180	194	194	204
NNSA Operating	155.0	163.5	146.7	124.6	117.8	120.1	113.9
NNSA Capital Equipment	1.7	1.1	--	--	--	--	--
Total National Nuclear Security Administration (NNSA)	156.7	164.6	146.7	124.6	117.8	120.1	113.9
Total NNSA Direct Personnel	310	247	241	246	261	263	275
Office of Energy Assurance (EA)							
Total Funding	--	0.6	0.6	0.6	0.6	0.6	0.6
Direct Operating Personnel	--	0.7	0.7	0.7	0.7	0.8	0.8
Office of Intelligence (IN)							
Total Funding	5.9	4.9	4.0	4.1	4.3	4.5	4.6
Direct Operating Personnel	26	20	20	21	21	22	22
Office of Counterintelligence (CN)							
Operating	13.2	14.3	13.3	13.5	14.0	14.3	14.5
Capital Equipment	--	--	--	--	--	--	--
Total Funding	13.2	14.3	13.3	13.5	14.0	14.3	14.5
Direct Operating Personnel	48	49	50	51	52	54	55
Capital Equipment Personnel	--	--	--	--	--	--	--
Assistant Secretary for Nuclear Energy							
Nuclear Energy R&D (AF)	1.2	0.8	3.1	4.4	3.9	5.6	5.6
Fast Flux Test Facility-FFTF (AF)	--	--	--	--	--	--	--
Isotope Production (ST)	0.1	0.0	--	--	--	--	--
Total Funding	1.3	0.8	3.1	4.4	3.9	5.6	5.6
Direct Operating Personnel	5	2	2	3	3	3	3

Table 7.5. Resources by Major DOE Areas (contd)

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Office of Security and Emergency Operations							
Nuclear Safeguards and Security (GD)	6.3	5.2	3.5	3.6	3.6	3.3	3.2
Safeguards and Security (FS)	9.9						--
Security Investigations (GH)	0.1	0.2	0.1	0.1	0.1	0.1	0.1
Emergency Management (ND)	--	--	--	--	--	--	--
Operating	16.2	5.4	3.6	3.6	3.6	3.3	3.2
Nuclear Safeguards and Security (GD)	0.4	--	--	--	--	--	--
Safeguards and Security (FS)	0.1	--	--	--	--	--	--
Capital Equipment	0.5	--	--	--	--	--	--
Total Funding	16.8	5.4	3.6	3.6	3.6	3.3	3.2
Direct Operating Personnel	20	19	19	19	20	20	21
Capital Equipment Personnel	0	--	--	--	--	--	--
Assistant Secretary for Fossil Energy							
Coal (AA)	3.8	6.4	7.1	8.4	10.8	11.6	12.4
Gas (AB)	1.2	0.6	--	--	--	--	--
Petroleum (AC)	0.2	0.0	--	--	--	--	--
Innovative Clean Coal Tech. (AZ)	0.0	--	--	--	--	--	--
Operating	5.3	7.1	7.1	8.4	10.8	11.6	12.4
Capital Equipment (AA)	0.3	0.3	--	--	--	--	--
Capital Equipment (AB)	--	--	--	--	--	--	--
Capital Equipment	0.3	0.3	--	--	--	--	--
Total Funding	5.6	7.4	7.1	8.4	10.8	11.6	12.4
Direct Operating Personnel	18	16	16	17	17	18	18
Capital Equipment Personnel	0	0	0	0	0	0	0
Office of Policy, Planning and Program Evaluation							
Policy, Planning, and Analysis (PE)	--	--	--	--	--	--	--
Total Funding	--	--	--	--	--	--	--
Direct Operating Personnel	--	--	--	--	--	--	--
Other DOE Organizations							
Total Funding	0.5	1.1	2.6	3.8	4.3	1.8	1.8
Direct Operating Personnel	3	6	6	6	6	6	7
Other DOE Sites							
Operating	17.4	16.2	11.6	11.7	11.8	12.2	12.6
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Total Net Funding	(38.9)	(46.8)	(44.4)	(47.4)	(48.4)	(50.0)	(51.6)
Direct Personnel	60	49	49	50	51	53	54
Total DOE Programs							
Operating	420.9	441.4	429.5	431.4	447.6	465.8	474.3
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Capital Equipment	14.0	9.1	8.9	11.8	12.1	14.4	14.7
General Purpose Equipment-GPE	--	--	1.0	1.0	1.0	1.0	1.0
General Plant Projects-GPP	6.2	4.8	4.0	4.0	4.0	4.0	4.0

Table 7.5. Resources by Major DOE Areas (contd)

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Total Funding	384.8	392.4	387.1	388.8	427.6	436.7	432.6
Direct Personnel							
Operating	1,233	1,190	1,194	1,226	1,256	1,288	1,326
Capital	3	4	4	4	4	4	4
General Plant Projects (GPP)	10	6	4	4	4	4	4
Construction Line Items	--	--	4	4	19	14	4
Total Direct Personnel	1,246	1,200	1,206	1,238	1,283	1,309	1,338
Work for Others							
Department of Defense							
Operating	25.7	42.0	50.8	52.2	54.8	57.2	59.1
Direct Personnel	87	127	96	135	137	139	142
Nuclear Regulatory Commission							
Operating	4.3	5.8	6.8	7.0	7.4	7.6	7.8
Direct Personnel	16	19	13	18	19	19	19
Environmental Protection Agency							
Operating	1.0	2.2	4.0	4.4	4.8	5.3	5.9
Direct Personnel	4	6	8	11	12	13	14
Dept. of Human and Health Svcs./NIH							
Operating	0.3	0.1	2.0	3.5	5.0	6.5	8.0
Direct Personnel	1	0	13	20	22	24	26
NASA							
Operating	0.1	0.2	0.8	0.8	0.8	0.8	0.8
Direct Personnel	0	1	1	2	2	2	2
U.S. Customs							
Operating	0.5	11.7	10.0	5.6	--	--	--
Direct Personnel	1.7	33.6	56.9	--	--	--	--
IRS							
Operating	3.9	0.3	4.0	4.0	4.0	4.0	4.0
Direct Personnel	12.0	0.6	7.6	10.3	10.0	9.8	9.6
Department of State							
Operating	0.4	4.1	0.7	--	--	--	--
Direct Personnel	0.3	8.4	1.3	--	--	--	--
Other Federal Agencies							
Operating	2.8	7.1	7.6	8.1	8.5	9.0	9.4
Direct Personnel	28	11	3	5	5	5	6
Other - Non-Federal Agencies							
Operating	2.1	2.3	5.9	5.9	6.4	7.0	7.7
Direct Personnel	8	2	11	16	17	17	17
Total Work for Others							
Operating	41.0	75.7	92.5	91.4	91.7	97.4	102.7
Direct Personnel	159	211	212	217	223	228	235

Table 7.5. Resources by Major DOE Areas (contd)

(Budget Authorization Dollar Amount in Millions)

	Fiscal Year						
	2001	2002	2003	2004	2005	2006	2007
Total Laboratory Funding							
Operating	461.9	517.1	520.7	521.5	538.1	562.0	575.7
Direct Personnel	1,392	1,401	1,406	1,443	1,479	1,516	1,560
Capital	14.0	9.1	5.9	8.8	9.1	11.4	11.7
Direct Personnel	3	4	4	4	4	4	4
General Purpose Equipment-GPE	--	--	4.0	4.0	4.0	4.0	4.0
General Plant Projects-GPP	6.2	4.8	4.0	4.0	4.0	4.0	4.0
Direct Personnel	10	6	4	4	4	4	4
Construction Line Items	--	--	1.0	1.0	24.3	14.9	4.0
Direct Personnel	--	--	4	4	19	14	4
Landlord Line Items	--	--	--	--	--	--	--
Direct Personnel	--	--	--	--	--	--	--
Indirect Personnel	1,381	1,423	1,441	1,458	1,485	1,507	1,526
Gross Laboratory Funding	482.1	531.0	535.6	539.3	579.5	596.3	599.4
Total Personnel	2,786	2,834	2,858	2,912	2,975	3,036	3,098
DOE Site Transfers and Cash Work	(56.3)	(62.9)	(56.1)	(59.2)	(60.2)	(62.2)	(64.2)
Net Laboratory Funding	425.8	468.1	479.5	480.1	519.3	534.1	535.3

Subcontracting and Procurement Awards

The Laboratory is dependent upon external resources (universities and industry) for support in achieving timely and successful completion of assigned programs and projects. This is accomplished by staff in the Business Support Services organization who use the procurement acquisition process in acquiring needed equipment, materials, supplies, and services. The table below reflects actual subcontracted amounts for fiscal year 2002 and projections for fiscal years 2003 through 2008.

Table 7.6. Subcontracting and Procurement							
(Dollar Amounts in Millions)							
	2001	2002	2003	Fiscal Year 2004	2005	2006	2007
Obligated	204.5	217.9	254.7	287.8	284.0	272.0	274.4
Subcontracting and Procurement from:							
Universities	17.3	27.6	30.6	34.5	34.0	32.6	32.9
All Others	161.7	158.8	192.3	217.4	214.6	205.4	207.3
Other DOE	25.5	31.5	31.8	35.9	35.4	34.0	34.2
Total External Subcontracts and Procurements	204.5	217.9	254.7	287.8	284.0	272.0	274.4

Socio-Economic Program Procurement Awards

The Laboratory is committed to support the socioeconomic objectives of DOE and has established procedures and programs that support meeting those objectives.

Table 7.7. Socio-Economic Program Procurement Awards							
(Dollar Amounts in Millions)							
	2001	2002	2003	Fiscal Year 2004	2005	2006	2007
Procurements from Small Business	35.5	59.8	59.7	67.7	66.7	63.9	64.5
Procurements from Disadvantaged Businesses	10.1	3.9	7.0	7.9	7.8	7.5	7.5
Procurements from Women-Owned Small Businesses	N/A	3.4	6.4	7.2	7.1	6.8	6.8
Procurements from HUBZone Small Businesses	N/A	8.8	2.6	2.9	2.8	2.7	2.7
Procurements from Veteran-Owned Small Businesses	N/A	N/A	0.6	0.7	0.7	0.7	0.7
Procurements from Service-Disabled Veteran-Owned Small Businesses	N/A	0.03	0.1	0.2	0.2	0.2	0.2

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Work for Others

Department of Defense

Pacific Northwest National Laboratory has been providing technology solutions to Department of Defense organizations for almost 40 years. We currently perform about \$38 million of research and development work each year for our Department of Defense clients. Primary sponsors include the Army, Navy, Air Force, Marine Corps, Defense Advanced Research Projects Agency (DARPA), the Defense Threat Reduction Agency, staff agencies within the joint and specified commands, and offices within the Office of the Secretary of Defense.

Laboratory research and development programs for Department of Defense clients address national security challenges posed by the asymmetric threat environment and force transformation imperatives of the 21st century. Our focus on solving the Department of Defense's "really hard problems" is reflected throughout the Work for Others portfolio and includes basic science work for DARPA and the Services' science and technology organizations, technology development to improve combat capabilities and weapons effectiveness, transform logistics operations, reduce the cost of facility operations, and remediate long-standing environmental insults at Department of Defense installations.

Research and development programs for Department of Defense clients employ and improve our capabilities in most of the Laboratory's skill areas, and complement and enhance our national security work for DOE. Some examples of the skills deployed on Department of Defense programs are analytical and physical chemistry, biosciences, biotechnology, computational science and engineering, computer science and information technology, design and manufacturing engineering, earth systems science, energy technology and management, human health and safety, materials science and technology, nuclear science and technology, policy and management sciences, sensors and electronics, separations and conversions, and statistics.

Following is a description of selected Work for Others programs for each of the major Department of Defense clients.

Defense Advanced Research Projects Agency

DARPA continues to support cutting-edge research and development at the Laboratory in many areas important to the security of the United States and relevant to the overall DOE mission. The Laboratory currently performs research for six of the eight DARPA Technical Offices. Some examples follow:

- *Information Exploitation* supports research in sensor and information systems technology and systems with specific application to battle space awareness, targeting, command and control, and supporting command post infrastructures. We are also developing advanced collaborative work environments in support of DARPA's Command Post of the Future Program.

- The *Special Projects Office* at DARPA sponsors our research on tactical multi-mode laser sensor systems, chemical weapons detection sensors, characterization of underground targets and facilities, and immune building systems.

Army

Army clients at Pacific Northwest National Laboratory include the Army Research, Development, and Engineering Commands; Army Research Laboratory; Army Forces Command; Army Logistics Integration Agency; Army Chemical and Biological Defense Command; and Army Communications and Electronics Command.

Following is a description of research and development programs at the Laboratory in support of Army clients.

- PNNL leads a major program to support the Army's Logistic Integration Agency in its efforts to implement Logistics Transformation.
 - We evaluate technology for application to the Army's logistics transformation goals, perform proof-of-principal demonstrations of promising technologies, develop inputs to the Army's science and technology master plan, and develop and maintain the Army's Strategic Logistics Plan.
 - We developed advanced prognostics technology and are crafting the master operational architecture needed to generate, transmit, and use data from embedded diagnostics and embedded prognostics systems on Army combat platforms.
 - We are making direct contributions to the development of doctrine, policy, and technology for the Army's Objective Force and Future Combat System program. We participated in technology identification and evaluation exercises conducted in the early stages of the Future Combat System program.
- Industrial base and organizational effectiveness assessments work includes technical support for modernization of major weapons production systems; evaluation of organization systems; procedures and methods, safety systems, and functioning of joint programs; and assessments of human factors, impacts, and training requirements.
- We are developing microthermal and microchemical systems that are of particular interest to the Army Research Lab. In these programs, we are developing compact microchannel chemical reactors and man-portable soldier systems (one is a compact personal cooling unit, and a liquid-hydrocarbon fuel processor to support man-portable power generation in a lightweight fuel cell). This research is joint with regional universities including Oregon State University and Spokane Intercollegiate and Technology Institute.
- Network architecture, distributed computing, and decision support techniques have been developed by Pacific Northwest National Laboratory to meet the specific needs of the Army Chemical Biological Defense Command and other federal and state emergency organizations. This Laboratory-developed system is deployed to each chemical weapons storage site, and is presently targeted to Homeland Security clients.
- PNNL provides an extensive array of environmental characterization and remediation technologies to Army clients. Army Corps of Engineers work

includes support of Columbia River efforts to balance salmon recovery, power generation and water use locally. Other work includes applying advanced remediation and pollution prevention technologies to increase sustainability of Army installations.

- PNNL as a DOE Federal Energy Management lead lab provides support to Army installations in evaluating and applying conservation technologies and implementing privatization initiatives to reduce cost of operation.
- A large transportable radar cross section measurement system is under development for the Army as follow-on to a long-standing program for the Army Aberdeen Test Center in radar cross section research and development and testing. This system will measure the radar cross section of combat systems for the Department of Defense Joint Signatures Office.
- We will continue to support the Army in advanced materials and design testing. The kinetic energy projectile project supports the design, analysis, testing, and development of advanced munitions and manufacturing techniques for the Armament Research Development and Engineering Center. PNNL is completing its development program for the depleted uranium penetrator used in the Army's current generation of kinetic energy anti-armor projectiles. We have transitioned the manufacturing process for the penetrators and transferred this technology to a commercial vendor.

Air Force

Air Force key clients at Pacific Northwest National Laboratory include the Air Force Material Command, Air Force Research Laboratory, and special agencies and centers supporting mission area requirements.

- U.S. Air Force is leading initial Department of Defense wide efforts to conduct an assessment of the potential for on-site electricity generation from solar, wind, and geothermal resources at military installations in the United States and Guam. PNNL is a major contributor, primarily on wind energy characterization including feasibility on various Department of Defense sites, impacts on the efficiency, reliability, and vulnerability of the installation's energy systems and regional cost/reliability impacts.
- Pacific Northwest National Laboratory continues to provide essential research and development and support services to Air Force Space Command in monitoring and assessing the low frequency radiation emanating from the three Pave Paws ground radar installations at Cape Cod, Nevada, and Alaska.
- Laboratory staff continue to provide the Air Force with unique analytical chemistry support and radionuclide applications development. We have very sensitive and high-precision analytical techniques to meet demanding measurement and testing requirements. The Laboratory has singular skills in analyzing radionuclides in support specialized Department of Defense needs.

Navy and Marine Corps

Navy and Marine Corps customers at Pacific Northwest National Laboratory include the Naval Air Systems, Naval Sea Systems (NAVSEA), Space and Naval Warfare Systems, Naval Facilities (NAVFAC), Office of Naval Research, Technical Support Working Group, and Marine Corps field installations.

Our research work for these clients has been primarily technology development to improve legacy system performance and efficiency, technology development to be inserted into future Navy infrastructure and systems, and developments that support the many aspects of information operations. Examples of research and development programs at the Laboratory in support of Navy and Marine Corps clients are as follows:

- Ultrasonic imaging systems have been developed and deployed in the field to monitor and evaluate airframe and munitions components. PNNL recently delivered an ultrasonic inspection system that is being used by the Navy and Air Force to inspect rocket motors for aging-related defects.
- The Laboratory recently completed several projects for private industry, NAVAIR, and as part of an internal research and development investment that expanded the capabilities of radio frequency identification technology. The Laboratory also developed and demonstrated an electronic “dog tag” based on this semi-passive radio frequency tag technology.
- PNNL developed an advanced prototype Turbine Engine Lubricant Analysis System that is installed and being tested on a front line U.S. Navy ship in a forward deployed environment. The underlying technologies/concept have been licensed to a local company for the manufacture of units for maritime, aeronautical, and terrestrial applications.
- The Laboratory, through its Marine Sciences Laboratory at Sequim, Washington, has developed and deployed environmental remediation technologies in terrestrial settings as well as analytical work in the aquatic environment to support NAVSEA and NAVFAC environmental security requirements.
- The Laboratory also performs fundamental chemistry modeling and material characterization research and development in support of NAVSEA using resources and expertise in the Environmental Molecular Sciences Laboratory and key resources in 300 Area facilities. These resources and expertise are also forefront in our work for the Office of Naval Research on advanced bio-pathogen sensor development.
- Our work for the Navy Criminal Investigative Service (NCIS) employs Laboratory expertise in information analysis through visualization applications. We also developed computer software for NCIS that will ensure a “secure” environment for their information processing and analysis requirements.
- PNNL works jointly supporting the National Counter Narcotics Center with the Hanford Hazardous Materials Management Emergency Response training facility. This important effort directly supports counter narcotics and counterterrorism programs.
- PNNL has begun a program to support the Office of Naval Research Expeditionary Warfare Energy science and technology program. Our energy technology experts evaluated lightweight and more energy-efficient technologies to support the U.S. Navy’s Transformation Roadmap. Future work is proposed in advanced fuel cell and solar technology.
- PNNL leads a joint Department of Energy/Department of Defense program to implement cost-effective energy efficiency and energy security technologies at Department of Defense installations. Examples include a combination of

off-the-shelf sensors, smart control systems, and condition-based maintenance techniques to dramatically reduce the operating costs for steam plants at three Marine Corps installations.

Defense Threat Reduction Agency

Pacific Northwest National Laboratory continues to support the Defense Threat Reduction Agency with primary emphasis on treaty monitoring, verification, and training of foreign border enforcement personnel at the Hanford Hazardous Materials Management Emergency Response training facility.

We are developing and delivering technology that enables real-time detection of chemical and biological warfare agents. We provide both classified and unclassified technologies to support treaty verification and on-site inspection programs.

Nuclear Regulatory Commission

Pacific Northwest National Laboratory's research and technical work supports each of the U.S. Nuclear Regulatory Commission's major program offices. This work covers all aspects of nuclear safety regulation.

Office of Nuclear Reactor Regulation

Pacific Northwest National Laboratory supports the Office of Nuclear Reactor Regulation's Division of Licensing Project Management with technical assistance for improving work processes and for staff reviews of operations safety issues and decommissioning-related activities. We also help to develop regulatory guidance and standard review plans for the nuclear facility decommissioning process. The Laboratory has also provided the Division of Licensing Project Management with technical support by reviewing emergency action levels and by developing emergency preparedness training for Nuclear Regulatory Commission inspectors.

We will continue to support the Division of System, Safety and Analysis in the area of commercial in-reactor fuel performance. This work includes technical reviews of vendor and utility submittals on fuel designs, fuel performance codes, and control rod assemblies. Our staff will also continue to assist the Commission, as requested, with on-site audits and inspection of fuel vendors and utilities.

We will continue to provide regulatory and licensing support to siting, operating license extension, and environmental protection areas, including the Environmental Standard Review Plan update and development effort. We will provide multidisciplinary managerial and technical expertise to assist the Nuclear Regulatory Commission with licensing reviews for operating reactors, for license extensions and early site permits, and for regulatory guidance updating activities.

Office of Nuclear Regulatory Research

Pacific Northwest National Laboratory staff will continue to provide technical assistance to the Office of Nuclear Regulatory Research in decommissioning analysis and regulation. Technical analysis and cost estimates are provided for decommissioning licensed nuclear reactor power plants and licensed fuel-cycle and other nuclear facilities. The support that we provide to the Nuclear Regulatory Commission on short-turnaround analyses and addenda to previous

decommissioning analysis reports will continue on a task-order basis. Current and future work will include periodic updates of the document NUREG-1307. These updates will reflect changes in the low-level waste burial site charge schedules. We also will reevaluate the earlier fuel-cycle and non-fuel-cycle facility reports to reflect current financial and regulatory conditions. We developed a new computer program for estimating decommissioning costs.

Nondestructive evaluation projects at the Laboratory provided the engineering databases that are needed to support the Commission's position and policy on regulatory guides, statements, analysis codes, and regulations. The elements of these projects included 1) studying nondestructive evaluation reliability to determine the effectiveness of in-service inspections, 2) optimizing in-service inspection programs using nondestructive evaluation reliability data and parametric fracture mechanics analysis to analyze and control risks, 3) assessing new nondestructive evaluation techniques and transferring technology to the regional offices and to the utility industry, and 4) developing a technical database for fabrication flaws in U.S. reactor pressure vessels for use in remaining-life predictions. The nondestructive evaluation technologies under study at the Laboratory include ultrasonics (including the synthetic aperture focusing technique for ultrasonic testing), eddy currents, and acoustic emission. We anticipate that we will have similar research roles as advanced reactor designs are developed and as applications for combined construction and operating licenses are submitted.

The Laboratory will continue to provide technical assistance to studies on low-level radioactive waste storage. This work will include classifying, characterizing, and assessing the characteristics of waste streams and activated metals, source terms for performance assessments, and chelating agents.

Pacific Northwest National Laboratory is one of the primary technical resources for the Nuclear Regulatory Commission on commercial nuclear fuel. Issues related to high-burn-up fuel in nuclear power plants have high priority. Our staff will continue to develop and revise two fuel performance computer codes. This work is closely related to the fuel work being done for the Office of Nuclear Reactor Regulation.

Office of Nuclear Material Safety and Safeguards

Pacific Northwest National Laboratory staff will continue to support research on chemical safety, security and safeguards, structural engineering, and international physical protection. Our staff also support the Spent Fuel Project Office in evaluating the performance of spent nuclear fuel casks. As the Department of Energy relinquishes additional fuel-cycle facilities to the Nuclear Regulatory Commission for regulation, we anticipate new opportunities to assist in reviewing and inspecting those facilities.

Other Nuclear Regulatory Commission Offices

Pacific Northwest National Laboratory continues to support the Nuclear Regulatory Commission's Incident Response Office by refining analytical tools used by the emergency response organizations. New and improved models that address cloud-shine, modify wind fields, process meteorological data, present results graphically, and calculate dose rates have been added to the RASCAL computer program. As this computer program is revised, tested, and installed, Commission staff are being trained on use of the program and code models.

Environmental Protection Agency

Pacific Northwest National Laboratory conducts research for the U.S. Environmental Protection Agency (EPA) to assist the agency in its central role of developing, implementing, and enforcing environmental regulations. This research focuses on ways to protect human health and the environment from chemical and non-chemical agents. This work is directly related to and complements our environmental science research for the Department of Energy. We continue to conduct a variety of research and development activities to improve our understanding of exposure, impacts, and risk to human health and ecological systems from environmental pollutants. The primary areas of research that we conduct for EPA include the following:

- measuring and analyzing the effects of toxic and hazardous chemicals on terrestrial and aquatic ecological systems, including the marine environment
- modeling and assessing the environmental impacts of increasing concentrations of trace contaminants, such as mercury and persistent organic pollutants (DDT, dieldrin), and associated air quality impacts
- modeling and analyzing hazardous waste transport and fate in soil, water (both fresh and marine), air, and biota
- assessing the technologies and economic impacts of selected international strategies to reduce greenhouse gas emissions
- developing human health risk assessment information, methods, and guidance, as well as improving the science and practice of risk assessment
- developing innovative compliance information tools for industry
- developing innovative pollution prevention design, management tools, and methods
- integrating disparate databases, disparate models, multiple-media models, and software-assessment frameworks
- assessing the impacts of global climate change
- developing and supporting new and innovative techniques for metals analyses and bioassays
- assessing endocrine disruption and receptor binding
- developing protocols for androgen and estrogen receptor binding
- assessing haloacid kinetics in mammals.

Pacific Northwest National Laboratory has developed capabilities to support EPA's risk-assessment priorities, including

- toxicology and dose-response relationships
- biological, ecological, and environmental field monitoring of toxic exposures and effects
- database and software development and quantitative modeling of exposure and risk
- exposure and risk interpretations and design of effective risk reduction strategies
- design and implementation of successful risk communication and outreach.

Pacific Northwest National Laboratory expects that the EPA will continue to support global climate research. We are involved in measuring and assessing the impacts of pollutants on ecosystems including the Arctic, Great Lakes, Everglades, and Northwest watersheds. Our researchers provide technical support to the environmental monitoring and assessment program by assisting in the design of studies to estimate on a regional basis the current status, extent, changes, and trends in indicators of the condition of the nation's ecological resources. We also provide technical support to the EPA's ocean disposal program by conducting bioassays of dredged material related to disposal area siting projects. The Laboratory also is developing and demonstrating methods and technologies for understanding and mitigating the risks associated with hazardous materials, such as the effects of contaminants on the reproductive health of humans and other mammals. The Laboratory supports a variety of EPA compliance and technical assistance programs. We also are involved in developing pollution prevention methods and tools, which go beyond compliance, for integrating environmental decision making into routine business practices, such as facility, product and process design, purchasing, and managerial accounting.

Pacific Northwest National Laboratory is cooperating with EPA Region 10 to support regional environmental activities. These activities include

- temperature and total-dissolved-gas assessments of the Columbia River and tributaries by developing a scalable database system for supporting water quality simulations
- regional air quality in the Columbia and Georgia Basins, including impacts to human health and the environment from agricultural, prescribed (silvicultural), wild, and other sources of burning over large areas of the Pacific Northwest
- arsenic analyses and mobility in soils at Superfund sites
- a cost-benefit analysis for contaminated sediment disposal of dredged material from the Puget Sound
- groundwater Total Maximum Daily Loads analysis and wellhead protection delineation
- commercialization of the EPA Region 10 Rapid Access Information Network System (a graphical database system) through an Environmental Technology Commercialization Center cooperative research and development agreement.

To coordinate these EPA Region 10 activities, we are exploring the formation of regional collaborative research centers, including

- Cooperative Institute for Air Quality and Health, which would represent a consortium of government, university, industry, and public researchers to support the cooperative study of air quality and related environmental effects in the Pacific Northwest region
- Northwest Natural Resources Breakthrough Center, which would be a center dedicated to solving long-term natural resources problems, serving government, industry, and nongovernmental organizations.

National Aeronautics and Space Administration

Pacific Northwest National Laboratory conducts research for the National Aeronautics and Space Administration (NASA). This work applies Laboratory

capabilities, developed in support of related DOE programs, to specific needs of NASA. This work is largely focused in five areas:

- Climate processes – we conduct modeling studies of the effects of atmospheric aerosols on the global thermal radiation budget, and we conduct research, development, and testing of satellite-based measurements of cloud properties.
- Satellite operations – we develop intelligent systems to monitor spacecraft functions and to automate small-satellite mission operations centers.
- Mars exploration – we develop microsystems for automated production of consumables on the Mars surface.
- Aircraft operations – we conduct statistical analysis of aircraft flight data and pilot reports for improving the safety and efficiency of commercial aircraft operations.
- Radiation dosimetry – we develop new radiation measuring systems for space flight applications.

Over the next several years, we will be expanding our research activities for NASA in the above focus areas. The Laboratory user facilities (Environmental Molecular Sciences Laboratory and Atmospheric Radiation Measurement) will be of particular value to these studies. In addition, we will be working to build stronger collaborations between the DOE and the NASA climate research programs.

In the future, we will be looking for new opportunities to apply our capabilities in microtechnology, information science, and nanoscience to NASA needs. We will continue to work with natural resource managers in the Northwest region to develop a Northwest collaboratory for natural resource management that will apply NASA remote sensing data to the solution of important resource management problems.

U.S. Department of the Treasury

Radiation Portal Monitoring Support to U.S. Customs. The U.S. Customs Service (USCS), Office of Information and Technology, Applied Technology Division, working with the Department of Energy (Pacific Northwest National Laboratory), has established a terrorist radiation/nuclear detection project to investigate systems and technologies to augment and enhance their existing radiological detection capabilities. This project addresses the maritime, aviation, land crossing, and rail USCS inspection environments. The Laboratory's scope of work includes documenting user requirements, conducting market surveys and technical performance assessments, providing specialized technical support, and deployment of commercial-off-the-shelf radiation portal monitors into USCS ports of entry.

Internal Revenue Service – Science and Technology Research and Development for Excise Tax Compliance. Pacific Northwest National Laboratory is supporting the Internal Revenue Service to develop an Excise Tax Compliance Program to administer excise fuel taxes and other excise taxes. Because the technical issues associated with fuel compliance are so different from the examination-based, case oriented functions that the IRS has traditionally performed, research is needed in a number of areas. Objective scientific methods are being developed to reduce the potential for tax evasion, detect tax evasion,

enhance compliance, better utilize IRS resources, and reduce the burden on legitimate taxpayers. Examples of significant and on-going contributions include:

- development of a prototype acoustic inspection device that can quickly differentiate taxable fuel products inside transport trucks
- development of rigorous fuel fingerprinting methods that can detect fuel adulteration, fuel blending, and track fuel back to its terminal source
- development of methods to detect and counter dyed fuel evasion schemes
- development of an economic model to predict fuel taxes
- development of data mining and analysis methods to better utilize IRS data
- development of improved training tools
- development of methods to detect ozone depleting chemicals on electronic circuit boards.

U.S. Department of Health and Human Services

The Pacific Northwest National Laboratory is involved in a significant level of research activity for the National Institutes of Health, most of which is performed under Battelle's Use Permit. In the future, where appropriate, research grant activity for the National Institutes of Health will be performed under provisions of the 1830 Work for Others contract mechanism.

Consistent with the Pacific Northwest National Laboratory's strengths in the biological and physical sciences, scientists perform multidisciplinary, collaborative research for the National Institutes of Health that integrates molecular biology, biochemistry, physics, mathematics, and computer science to advance our understanding of complex biological systems. The Environmental Molecular Science Laboratory and Pacific Northwest National Laboratory's forefront program in microbiology provide an integrated multidisciplinary environment for research staff and a set of exceptional tools for the study of complex problems in a broad range of biological systems. During the past decade the Laboratory has invested in systems biology capabilities that build on and extend the one-of-a-kind facilities and instruments in the Environmental Molecular Sciences Laboratory. We have built a significant program in proteomics and have demonstrated leadership in high-throughput mass spectrometry. We are also developing the next-generation instruments for direct observation of chemical and physical processes in living cells. The National Institutes of Health provide funds for research in a variety of areas which include mechanistic studies of cellular processes, the development of methods and instruments for proteomic analysis, NMR structural studies of biomolecules, and computational biology and informatics.

Other Federal and Nonfederal Agencies

A number of other federal agencies fund work at Pacific Northwest National Laboratory. They include the Department of Transportation, Department of Justice, Federal Bureau of Investigation, United States Forest Service, and Department of Commerce. Work for non-federal entities includes funds from Washington State, Fred Hutchinson Cancer Research Center, and King County (Washington) Department of Natural Resources.

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University and Industrial Partnerships and Collaborations

University Partnerships and Collaborations

Partnerships between the Department of Energy's national laboratories and universities strengthen our nation's intellectual and economic competitiveness. Pacific Northwest National Laboratory is 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 are pursuing a Collaborative Institute for Bioproducts Research with Washington State University, University of Idaho, and the Idaho National Engineering and Environmental Laboratory. Other partners may participate, including the U.S. Department of Agriculture (Western Region) and the University of California at Davis. This collaborative institute will focus on the comprehensive use of agricultural materials for producing a broad spectrum of products - from pharmaceuticals to commodity chemicals. Research will include development of new crops for production of high-value products, development of biological processing and catalysis systems for production of commodity chemicals, and systems for separating product species.

Carbon Management and Climate Studies

Carbon management is a combination of studies in a variety of fields, including atmospheric, oceanic, terrestrial, technological, economic, and social sciences. Pacific Northwest National Laboratory is a primary participant in the nation's two largest research and development consortia focusing on terrestrial carbon sequestration.

The Consortium for Agricultural Soils Mitigation of Greenhouse Gases provides tools and information needed to sequester carbon dioxide and provide incentives for improving farm soil. Benefits include an increased and stable agricultural production and an overall reduction of soil erosion and pollution by agricultural

chemicals. The Consortium brings together the nation's top researchers in soil carbon, greenhouse gas emissions, conservation, computer modeling, and economic analysis. Partners include Colorado State University, Iowa State University, Kansas State University, Michigan State University, Purdue University, Ohio State University, Texas A&M University, and the University of Nebraska.

The Carbon Sequestration in Terrestrial Ecosystems Research and Development Consortium characterizes pathways and mechanisms for creating larger, longer lasting carbon pools in terrestrial ecosystems. Pacific Northwest National Laboratory and Oak Ridge National Laboratory lead this effort. Partners include Colorado State University, Kansas State University, North Carolina State University, Ohio State University, Texas A&M University, the University of Washington, and Washington State University.

We collaborate with Battelle-Columbus Laboratories, BP (formerly British Petroleum), American Electric Power, Ohio State University, and West Virginia University to characterize the geology of the Ohio River Valley and better understand the potential for geologic sequestration of carbon dioxide in this region. We are also working with the University of Alaska at Fairbanks and BP on an effort to use carbon dioxide to enhance the production of methane from methane-hydrate-bearing formations in Alaska.

In 2001, the Laboratory formally established the Joint Global Change Research Institute with the University of Maryland to conduct multidisciplinary research in various topics related to the scientific and policy study of global energy and the environment. The Joint Institute is focused on three areas: leading the development of integrated assessment approaches to climate change, the establishment of energy efficiency centers and the creation of nontraditional funding mechanisms for energy projects, and understanding both the effects of climate change and the associated social vulnerabilities these effects may create. The move to the University was engendered by the expectation that the assets of the University could enhance each of the existing major program areas. In particular, the departments of demography and geography and the School of Agriculture and Natural Resources have capabilities not replicated at Pacific Northwest National Laboratory or even in the rest of the DOE laboratory system. Further, the University's strong connections to nearby National Aeronautics and Space Administration and National Oceanic and Atmospheric Administration laboratories increases the opportunity for the Institute to interact more effectively with these two key partners in the United States Global Change Research Program.

More than 20 other universities partner with the Laboratory in the Atmospheric Radiation Measurement program, which addresses some of the great uncertainties about greenhouse gases and their potential impact on global climate. We collaborate with the University of Washington on research to predict the impacts of climate change and variability on water resources in the western United States. A joint project with the University of Arizona seeks to develop and apply regional climate and hydrologic models for semiarid regions, such as the southwestern United States. We work with the University of California at Berkeley on coupled land-atmosphere models to account for land surface heterogeneity and its effects on the atmosphere. We collaborate with Oregon State University on a joint study on the impacts of climate change on vegetation and with Washington State University to develop models for climate change impacts on crops. We work with the State University of New York at Albany on an intercomparison of regional climate models

over East Asia. We collaborate with the Georgia Institute of Technology to estimate radiative forcing of tropospheric aerosols. Also, we are studying the climatic effects of El Niño and La Niña on agricultural production and water resources in the United States in joint research with the University of Florida.

Computer and Network Infrastructure Security

Pacific Northwest National Laboratory is collaborating with the University of Idaho on computer hardware, software, and network infrastructure security. The University of Idaho has efforts under way to develop secure and dependable software to detect and deter intruders, preserve information integrity, and improve the quality and security of electronically mediated interactions.

Computational Sciences

As a national scientific user facility, the capabilities of the William R. Wiley Environmental Molecular Sciences Laboratory are available to outside researchers after full peer-review of research proposals. Active research collaborations in theory, modeling, and simulation involve scientists from about 80 colleges and universities in the United States and about 60 universities representing 30 countries. As another measure of collaboration, more than 250 sites use our Molecular Sciences Software Suite (MS³). New efforts include development of a Collaboratory for Multi-Scale Chemical Sciences with the Massachusetts Institute of Technology, the University of California, Berkeley, and other DOE laboratories that will take an informatics-based approach to enhance coordination of research efforts across related subdisciplines in chemical sciences, and also will enhance our ability to meet DOE's national research challenges.

Laboratory scientists work with computational scientists at the University of Washington on methods to predict the behavior of waste storage glasses. Collaborations with the University of California-San Diego are yielding CarParinello ab initio molecular dynamics codes. The MS³ software is being used for molecular dynamics simulations of proteins associated with Alzheimer's disease and acquired immunodeficiency syndrome. A substantial, long-term collaboration with Washington State University will develop quantum chemical methods and new correlation-consistent basis sets. We work with the University of Southern California and Phillips Air Force Research Laboratory on fluorine chemistry, including studies on basicity and acidity scales. Research with Columbia University is leading to the development of new force field parameters for biomolecular and separation systems. We work with the University of Houston on studies of biomolecular interfaces, notably DNA-chip arrays, and on simulating the sedimentation of biomolecular assemblies. In collaboration with Ohio State University and Stevens Institute of Technology, we are developing relativistic quantum chemical methods to predict the properties of actinide complexes critical to the environmental management effort of the Department of Energy. A long-term collaboration with the University of Minnesota will develop new theories of chemical reaction rates in the gas phase and in solution.

We work with the Massachusetts Institute of Technology and the University of Colorado-Denver in applied mathematics and computational biology. An active collaboration with Oregon Health & Science University involves computational chemical studies of the chromophores that serve as biomarkers for neurotoxins.

We have strong interactions with the Georgia Institute of Technology in studies of porous silicon. We collaborate on computational chemical methods with Texas A&M University, the University of Utah, the University of Utrecht (The Netherlands), and the University of California at Berkeley. We collaborate in computational chemical applications with McMaster University (Hamilton, Ontario), on studies of inorganic complexes involving fluorine, and with the Autonomous University of Mexico-Iztapalapa on hydrogen bonding and new density functional theory approaches.

Along with several other university and Laboratory partners, Pacific Northwest National Laboratory is active in DOE's program called Scientific Discovery through Advanced Computing. The Scalable Systems Software Center provides tools for effective management and use of terascale computing resources, and includes partnerships with the University of Illinois (Urbana-Champaign), and with other DOE national laboratories. The Terascale Simulation Tools and Technologies Center provides technologies to enable application scientists to easily use multiple mesh and discretization strategies within a single simulation on terascale computers, in a partnership with State University of New York-Stony Brook, Rensselaer Polytechnic Institute, and other DOE laboratories. The Center for Component Technology for Terascale Simulation Software involves research into software component technology for high-performance parallel scientific computing to address problems of complexity, reuse, and interoperability for simulation software, and is being developed in conjunction with Indiana University, the University of Utah, and other DOE laboratories. In another DOE computing research program, the Center for Programming Models for Scalable Parallel Computing is a large collaborative effort with the University of Houston, University of Delaware, Rice University, University of Minnesota, Ohio State University, California Institute of Technology, University of Illinois, University of California at Berkeley, and other DOE laboratories.

Environment and Health

Pacific Northwest National Laboratory and Oregon State University participate with the Oregon Health & Science University's Superfund Basic Research Center to explore the effects on the nervous system of environmental pollutants that contaminate water supplies. The objective of this research is to improve assessment of exposure to populations adjacent to Superfund sites. This research involves the use of real-time breath analysis and physiologically based pharmacokinetic modeling to measure and describe dermal, oral, and inhalation exposure of residents located adjacent to Superfund sites. Pacific Northwest National Laboratory is working with a team of students in Evergreen State College's Student Oriented Software program exploring distributed computing technologies to improve the execution speed of PC-based computational models, using as a model system the Laboratory's Distributed Hydrology Soils Vegetation Model.

Pacific Northwest National Laboratory is collaborating with the University of Idaho's Water Resources Research Institute, Oregon State University Center for Water & Environmental Sustainability & Institute for Natural Resources, and State of Washington Water Research Center to deliver an integrated science and technology program for the development of tools and understanding leading to improved management of Pacific Northwest regional water.

Imaging Science and Technology

Pacific Northwest National Laboratory is collaborating with the University of Washington's Human Interaction Technology laboratory to develop new methods for enabling humans to visualize and interact with three-dimensional data sets. A collaboration with Pennsylvania State University focuses on development of flexible architecture for integrating multiple image analysis tools. Joint proposals and student internships are being conducted with Utah State University in the field of image analysis and software development. Under a recent collaboration with Central Washington University, the Laboratory and the university will explore and develop new methods for integrating distributed, diverse imagery databases using software agents.

International Security and Nonproliferation

Pacific Northwest National Laboratory and the University of Washington have established the Institute for Global and Regional Security Studies. The three principals are the university's Jackson School of International Studies and Department of Political Science and the Laboratory's Pacific Northwest Center for Global Security. The Institute is intended to promote greater understanding within the Pacific Northwest of issues affecting the national security of the United States, and to expand Pacific Northwest National Laboratory's capacity to serve its DOE client base by providing greater access to the academic community. In its first 18 months, the Institute has initiated an entirely new academic curriculum on security studies, sponsored colloquia and conferences, and started a new publication series on international security.

Princeton University and the University of California at Los Angeles contribute their expertise to the Laboratory's research on micro-electromechanical and nanolithography technology, and to our development of micro-laser transmitter arrays for infrared chemical sensing. We also collaborate with the University of Idaho to develop methods for detecting trace chemical vapors by infrared absorption spectroscopy. The Laboratory also collaborates with Washington State University on studies of cadmium zinc telluride, a semiconductor material used in solid-state gamma-ray spectrometers. These technologies are important for nuclear arms control, nonproliferation, and verification activities vital to national security.

Life Sciences

The Cell Systems Institute partnership agreement between the University of Washington's School of Medicine and Pacific Northwest National Laboratory was completed in 2001. The focus of this joint program is on coupling theoretical and experimental studies of cell-signaling components of the dynamic information control systems in cells. Other collaborative efforts in systems biology are under way with the Massachusetts Institute of Technology, the University of California at San Diego, and the University of Utah.

We collaborate with the University of California at San Diego and with the University of Arizona on single-molecule studies of ion-channel membrane receptors and other trans-membrane phenomena. We collaborate with Harvard University on studies of adaptive response and bystander effects for low-dose exposures to

low linear energy transfer ionizing radiation. We also work with scientists at the University of Texas at Austin on the role of prostaglandins in oxidative stress after exposure to contaminants. We support the University of Washington and the Fred Hutchinson Cancer Research Center (Seattle) with medical internal dosimetry for two major, long-term clinical studies on advanced treatment of lymphoma and leukemia using high-dose radiolabeled monoclonal antibodies.

Nanoscience, Nanotechnology, and Microtechnology

The rapidly developing field of nanoscience and nanotechnology will require active collaborations with university researchers in materials science, chemistry, bioengineering, and computations. In 2001, we established a Joint Institute for Nanoscience with the University of Washington for joint research on particles, films, and nanoclusters for a variety of applications, as well as chemically specific imaging at the nanoscale. Our strengths in synthesis, materials characterization, nanobiology, and computation will match well with the University of Washington's strengths in bioengineering and medical sciences. Additionally, a collaborative effort between the University of Washington and Pacific Northwest National Laboratory has been funded through the National Science Foundation to support the creation of new coursework, incorporating distance-learning tools, in various nanoscience and nanotechnology areas.

The Laboratory also established a Microproducts Breakthrough Institute with Oregon State University. This collaboration is designed to develop and help market advances of microtechnology in the Pacific Northwest. The institute is expected to help create a new and important industry which boasts smaller, lighter, and more efficient microtechnology-based energy, and chemical and biological systems for commercial and non-commercial use. The institute is centered at Oregon State University, but draws upon equipment, facilities, and staff from both organizations.

Nuclear Energy

The Laboratory is collaborating with the University of Texas Nuclear Engineering Program on a DOE Nuclear Energy Research Initiative proposal for a 3-year study to develop shielding materials for advanced light-water reactor pressure vessels. With the University of California at Berkeley, we are developing an advanced nuclear fuel capable of achieving extended burnup without any of the deleterious effects observed in present fuels. The objective of this research is to create a fuel, based on the presently licensed uranium oxide fuel, that contains various dopants that will stabilize the fuel matrix, increase retention of fission products, and improve thermal properties. Candidate materials are developed and tested at the Laboratory, using staff and visiting graduate students, and modeling activities are performed at the university.

Pacific Northwest National Laboratory conducts joint research with the University of Michigan to investigate radiation-induced changes in structural materials and the influence of these changes on materials performance in current and advanced nuclear power reactors. We also collaborate with the University of Illinois to evaluate basic mechanisms of interfacial deformation in materials. The Laboratory is also working with Ohio State University, Oregon State University, and the University of Utah on ways to increase the number of nuclear engineers, technicians, radiochemists, and health physicists.

Remote Sensing Applications

Pacific Northwest National Laboratory is leading the development of the Northwest Energy Technology Collaborative. Initial participants include the Idaho National Environmental and Engineering Laboratory, the University of Washington, Idaho State University, the University of Idaho, and Oregon State University. This Collaborative will serve as a platform to improve the delivery of remote sensing and related spatial information technologies and applications from developers to end users. Applications encompass environmental planning and natural resources management, emergency planning and response and homeland security, agriculture, and urban planning and development. The Collaborative will deploy advanced on-line collaboration tools, outreach and extension services, and advanced research and development in sensor technology, image processing, applications modeling, and data management and archiving.

Waste Characterization and Management

Our Laboratory collaborates with several universities to solve one of the highest priorities at the Hanford Site – the safe disposal of more than 50 million gallons of highly radioactive waste. Laboratory staff collaborate with Washington State University and Yale University to develop strategies for treating Hanford tank waste. Another project with Washington State University employs laser ablation and mass spectrometry to analyze the material composition of tank waste. We work with the University of Idaho on waste sequestration and sonic methods for detecting plugs in waste transfer pipelines. We collaborate with Texas Tech University on oxidation pathways in organic ion exchange media. Laboratory staff collaborate with the University of California-Santa Barbara on studies of molecular recognition and separation technologies using mesoporous materials.

Pacific Northwest National Laboratory collaborates with Washington State University and Montana State University on the Natural and Accelerated Bioremediation Research program to stop the movement of toxic metals in groundwater. This project specifically targets lead and uranium, the two most common radioactive and metallic contaminants in soil and groundwater at DOE facilities. Also, the Laboratory, New Mexico State University, and Florida State University collaborate on bioremediation of hexavalent chromium in the unsaturated zone to prevent future contamination of groundwater. Our staff collaborate with scientists at the Oregon Health & Science University and Oregon State University on pollutant toxicity associated with contaminated water supplies. This team is investigating ways to remove contamination, prevent toxic health disorders, and promote community and workplace health. We also collaborate with the University of Michigan on a study that has developed methods for immobilizing excess plutonium in gadolinium zirconate.

The Laboratory and Oregon State University collaborate on a DOE Environmental Management Science Program project examining interactions between microbiological and hydrological processes in the unsaturated zone. The objectives of this research are to develop methods to stimulate bacterial growth and colonization in the unsaturated subsurface to support bioremediation of contaminants, and to improve numerical fate and transport models in the unsaturated zone by including microbiological processes.

Pacific Northwest National Laboratory has been collaborating for more than 20 years with researchers at the University of Michigan on radiation effects in nuclear waste forms. This work has focused recently on radiation-resistance materials for the immobilization of nuclear materials and nuclear waste – recognized by the DOE Office of Science as one of the top 101 discoveries in the past 25 years.

Instrumentation and Students

The Laboratory supports regional colleges and universities through our equipment loan program for used equipment at the Laboratory. This allows faculty access to sophisticated instrumentation for performing research and for teaching. The equipment loan program also builds collaborations between regional faculty and Laboratory staff. Over 100 pieces of laboratory equipment and computers are currently on loan to regional colleges and universities. This equipment ranges from desktop computers to microscopes to mass spectrometers. Because of the rapid advancements in computing, most of our loaned, used computers are eventually donated to colleges and universities. Equipment such as spectrometers, microscopes, and centrifuges are often used in teaching laboratories.

The Laboratory hosts summer and semester students from regional colleges and universities. These “hands-on” experiences give regional students insight into future science and engineering careers. When possible, we provide appointments and mentoring for underrepresented students in science and technology.

For the last few years, the Laboratory has sponsored student teams from Seattle University. These teams are composed of seniors in computer science and engineering. A Laboratory staff mentor works with the students and their faculty advisor to complete a project specified by the Laboratory. Two projects are under way this year. One project is sponsored by our statistics group and involves aviation safety. The students are taking digital data collected from many different sources onboard the aircraft to identify typical flight patterns and atypical flights. A second team of students is working with intelligent agents that are used to mine information from large sources of data. In particular, they are developing an agent control environment that allows a nontechnical user to do data search and retrieval on the World Wide Web. These projects are a wonderful opportunity for the students and promote a positive image of the Laboratory in the university community.

Heritage College

Heritage College is a small, liberal arts college in Toppenish, about 70 miles west of Richland. Heritage serves a nontraditional student population (predominantly women, Hispanics, and Native Americans) long known for being underrepresented in higher education.

Several Laboratory scientists and managers actively support Heritage College in a variety of ways. One of these is guidance regarding the development of a horticultural initiative in the cultivation and propagation of native plants, and the Laboratory provided a greenhouse for that purpose. The Laboratory donated a mass spectrometer and gas chromatograph to enhance analytical capabilities in chemistry, biology, and environmental sciences. The Laboratory provides 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

In September 2001, the Oregon University System, Oregon Health & Science University, and Pacific Northwest National Laboratory signed a Memorandum of Understanding to form a cooperative relationship for research and educational activities. The Oregon University System includes Eastern Oregon University (La Grande), Oregon Institute of Technology (Klamath Falls), Oregon State University, Portland State University, Southern Oregon University (Ashland), the University of Oregon (Eugene), and Western Oregon University (Monmouth). Oregon Health & Science University includes the Schools of Dentistry, Medicine, Nursing; the Oregon Graduate Institute School of Science and Engineering; Oregon Health & Science University Hospital and Doernbecher Children's Hospital; many primary care and specialty clinics; and public service and outreach units. Among the areas of initial focus will be collaborations in the life sciences, physical sciences, and economic development.

The Northwest Virtual Entrepreneurial Support Network will be established to share technology, management, money, and marketing resources in Oregon and Washington in an effort to create successful high-tech businesses. The network will identify, develop, and commercialize intellectual property derived from the partnership. Partners are Pacific Northwest National Laboratory and the Oregon Technology Transfer Council, which comprises the technology transfer officers from Oregon's research universities.

Future collaborations will include educational and training opportunities, staff and faculty development programs, short courses and conferences, and visiting scientist programs in addition to collaborative research and jointly operated research institutes.

Washington State University, Tri-Cities

The local support by Laboratory staff members is essential to the success of the Washington State University branch campus in Richland. Laboratory staff members teach regular undergraduate and graduate courses, mostly during the evening, in a wide variety of subject areas. Staff members also teach short courses in the Professional and Continuing Education program at Washington State University.

In 2001, a new faculty member joined Washington State University, Tri Cities, with the support of Pacific Northwest National Laboratory, to create a collaborative program in systems biology. The first master's degree candidates are expected to enroll in the fall of 2002, and a doctoral program is in the planning stages.

The Consolidated Information Center houses the library facility at the branch campus in Richland. The Center also houses the Hanford Technical Library and the DOE Public Reading Room (both operated by Pacific Northwest National Laboratory). The Hanford Technical Library and the DOE Public Reading Room are collocated with the Washington State University, Tri Cities branch library in the section of the building called the Consolidated Libraries. Additionally, the Consolidated Information Center provides space for a Life Sciences Laboratory, museum space, and conference rooms that are available to DOE and contractors.

In summary, Pacific Northwest National Laboratory maintains active collaborative relationships with hundreds of colleges and universities. Laboratory-university partnerships direct complementary capabilities and resources toward common

priorities for enhancing our quality of life and protecting and preserving our environment. These relationships promote shared interests in research, education, and professional and economic development, and they bring new intellect, insights, and inspiration to our common focus on significant issues and opportunities.

Industrial Partnerships and Collaborations

Science discoveries at Pacific Northwest National Laboratory often produce innovative technologies with outstanding commercial value. Pacific Northwest National Laboratory participates with private industry, other national laboratories, and government and private research institutes in the United States and abroad on a large number of scientific research and engineering studies. We provide access to project-oriented scientific teams, outstanding user facilities, and instruments and tools for collaborative research and development in support of a broad range of technologies. These partnerships create opportunities for cost-effective research and ways to license promising new technologies. Among the Laboratory's major industrial partners are General Electric Company, Motorola, Delphi Engineering Group, Weyerhaeuser Corporation, Ford Motor Company, General Motors, PACCAR, Freightliner, E.I. DuPont de Nemours, Caterpillar, Boston Scientific Corporation, Sharp Microelectronics, Sawtec, Inc., IBM, Berkeley Instruments, Tektronix, and Molelectron Detector, Inc.

The Department of Energy's Office of Science 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 application over a broad spectrum of scientific disciplines such as advanced materials science, intelligent chemical processing, efficient manufacturing, sustainable environmental technology, and innovative biotechnology.

The Laboratory also works with and supports 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. This program on global climate seeks 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. This program has broad participation by the DOE multiprogram national laboratories, several universities, and industrial participants.

In our **environmental quality** mission, we participate actively in the Environmental Management Science Program. The focus of the Laboratory's projects under this program is 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. We also worked with Fluor Hanford on 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.

We work with the Department of Defense, State Department, the Defense Threat Reduction Agency, and the U.S. Customs Service International Border Security Training. This program provides comprehensive training for border enforcement officials to better detect, identify, investigate, and interdict smuggling activities.

The Foundation for Russian American Economic Cooperation is a strategic Laboratory partner. The partnership dates to the origins of the Nuclear Cities Initiative when the Laboratory recruited the Foundation to serve 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. The Foundation continues to work with Pacific Northwest National Laboratory on other Nuclear Cities projects, including delivery of equipment to the city of Zheleznogorsk, helping the city of Zheleznogorsk on a strategic down-sizing plan, and working with the city of Zheleznogorsk to set up a new software development company.

Under the direction of George Russell, the former president of the Frank Russell Company, and Chairman of The Russell Family Foundation, the Laboratory has received assistance on Russian economic matters related to our fostering of a worldwide initiative to swap Soviet-era Russian Federation debt for programs on nonproliferation. This work also was a result of a partnership formed with the Nuclear Threat Initiative, which provided funding to Battelle Pacific Northwest Division to study the implementation of a Russia nonproliferation debt fund.

The National Bureau of Asian Research and the Laboratory have entered into a strategic alliance under the auspices of the Laboratory's Pacific Northwest Center for Global Security. Pacific Northwest National Laboratory 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 the sponsorship of the Laboratory, 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 energy 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. The Laboratory is 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. The Laboratory will participate in the Massachusetts Institute of Technology's Consortium on Protocols for Dynamic Energy Control. Pacific Northwest National Laboratory will assist Utility Automation Integrators, Inc. in the design and enhancements of the uaDispatch 2.0 product, select a site for implementation of the outage management system demonstration in Alabama, and deploy an operational system at the site. This system allows for visual display of outages and dispatch of crews to the most likely source of the problem causing the outage. The expanded capabilities will increase the scalability of the system and allow it to serve utilities nationally.

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 the Department of Energy's goal of advancing the development and sales of highly efficient new and emerging technologies. Successful initiatives have focused on compact fluorescent lamps and fixtures and rooftop air conditioners.

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, Daimler-Chrysler, and Cummins Diesel. These programs also support DOE's transportation focus in

government industry partnerships in FreedomCAR and 21st Century Truck. The immediate mission is to assist the Partnership for a New Generation of Vehicles, a Presidential initiative.

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, the Idaho National Engineering and Environmental Laboratory, 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 **biotechnology**, the DOE Laboratory Technology Research program funds partnership projects between the Office of Science national laboratories and private-sector companies. These partnerships benefit the participating companies and help achieve DOE mission responsibilities. Projects are funded in areas where the laboratories have state-of-the-art scientific capabilities, such as materials sciences, biotechnology, analytical chemistry, and advanced computing. For example, the Laboratory recently teamed with Genometrix, Inc. (The Woodlands, Texas) under the Laboratory Technology Research program to develop an automated system for detecting pathogens in the environment by purifying and amplifying DNA from sediment, soil, and aerosol samples and food extracts.

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 Chernobyl Unit 4 reactor. We plan to partner with nuclear engineering companies that are developing the next generation of modular nuclear reactors.

C

Laboratory Directed Research and Development

Laboratory Directed Research and Development (LDRD) at Pacific Northwest National Laboratory is an important mechanism for ensuring the future strength of our research and technology development capabilities. It is our principal means for supporting exploratory concepts, innovative approaches, and advanced studies needed to solve the most challenging scientific problems. The principal objectives of the Laboratory's LDRD program are to

- enhance our ability to address current and future Department of Energy missions
- maintain the Laboratory's scientific and technical viability over a broad range of disciplines
- foster creativity and stimulate exploration at the forefronts of science and technology
- serve as a proving ground for new research concepts
- support high-risk, potentially high-value research and development.

LDRD Program Benefits to DOE and to the Laboratory

The LDRD program increases the value that Pacific Northwest National Laboratory provides to the Department of Energy as a multiprogram national laboratory. Many of the Laboratory's best scientific ideas were developed with LDRD funds and are now providing support 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 Pacific Northwest National Laboratory remains a modern research facility well into the 21st century.

Institutional and Mission Areas of Emphasis^(a)

The LDRD program supports new and innovative projects in each of the four research directorates at the Laboratory – Fundamental Science, Environmental

(a) For additional detail on FY01 LDRD project accomplishments and costs, see PNNL's FY01 LDRD Annual Report. PNNL's FY02 LDRD Annual Report will be published in March 2003.

Technology, Energy Sciences and Technology, and National Security. Projects cross organizational boundaries and link staff with similar expertise and research interests. Approximately 70 percent of the projects are strategic, Laboratory-level projects, directed at developing capabilities in support of one or more mission areas. Approximately 30 percent of the projects are directorate-level projects that support directorate-level mission areas and priorities.

In line with our vision, the following major thrust areas for fiscal year 2003 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.

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 nano-biology. 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.

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 Pacific Northwest National Laboratory’s key research areas, including atmospheric chemistry and transport, complex biological processes, subsurface science, and materials engineering and simulations.

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 Department of Defense. Research supporting homeland security focuses on two areas. The first area is the development of “smart materials” that provide rapid, selective detection of threat chemical, biological, and nuclear materials. The second thrust area is the development of new analytical, statistical and computational methods to acquire and manage large, diverse information streams and then discover linkages and patterns in that information that may be indicators of potential terrorist actions. 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, dynamic characterization of cellular processes and characterization of engineered materials.

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, biobased products, and processes for energy-intensive industries.

Clean, Secure, and Affordable Energy—In this area, our research is focused on advanced power systems using solid oxide fuel cell technology for widespread applications in vehicles and buildings. This research seeks to overcome the limitations of high-temperature operations, improve component manufacturing, and improve system performance. We are also 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.

There were a number of noteworthy accomplishments in fiscal year 2002 on specific LDRD projects, highlighted below. These projects can be mapped to specific mission areas above.

- **Cell Signaling**—We developed a technique for studying ion flux across cell membranes in living cells to determine how cells respond to their environment. From these results, we formulated predictive models of cell-signaling pathways and networks to better understand intracellular function and responses to external stimuli.
- **Proteomics**—We used advanced separation sciences techniques involving protein arrays and high-resolution chromatography, combined with mass spectrometry, to show how proteins are organized into pathways and networks, and how proteins interact to form functional complexes. Functional proteomics has important applications in systems biology, new drug development, and in national security in areas such as identifying signatures of biological warfare agents.
- **Carbon Sequestration**—We developed a novel concept for simultaneous injection of carbon dioxide and production of methane hydrates. We proved that injection of carbon dioxide into geologic basalt formations results in-situ mineralization of the carbon dioxide, and made extraordinary progress in the development of computational tools for analyzing the fate- and effects of carbon dioxide that is injected into deep saline sedimentary formations. Each of these three accomplishments have the potential to have a major impact on the directions of DOE programs and the opinion of the scientific community in these areas.
- **Scalable Computer Algorithms**—We developed high-performance, scalable computer algorithms for analyzing multiphase atmospheric processes. We also developed mathematical techniques for large-scale data archive and scientific data management.

- **Aerosol Analysis Mass Spectrometry**—We modified a conventional laser desorption ion trap mass spectrometer for chemical analysis of aerosol particles. This system is being tested at the Hanford Site as a method to analyze samples and detect potential tank leaks more quickly and at lower cost.
- **Nanoscale Materials Technology**—We discovered and characterized new nanocrystalline metal oxide materials. We developed and tested novel photocatalysts grown as copper oxide quantum dots on anatase substrates for applications such as hydrogen production. We produced molecular beams to synthesize and characterize nanoporous magnesium oxide thin films with high surface areas.

Peer Review and Self-Assessment

Pacific Northwest National Laboratory uses technical 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, which includes an annual and midyear review, uses 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.

Summary

The LDRD program is a key factor in the Laboratory's ability to renew and strengthen signature capabilities and to respond rapidly to new scientific challenges resulting from DOE missions. 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.

LDRD is funded through a Laboratory overhead account applied to the value-added base for all Pacific Northwest National Laboratory 1830 Contract accounts, and represents approximately 3 percent of the Laboratory’s total operating budget. A total of 136 LDRD projects were supported during fiscal year 2001 (*Laboratory Directed Research and Development Annual Report, Fiscal Year 2001*, PNNL-13855, Pacific Northwest National Laboratory, Richland, Washington, April 2002).

Laboratory Directed Research and Development Funding (Budget Authorization Dollar Amount in Millions)							
FY 2000	FY 2001	FY 2002	FY 2003	FY 2004	FY 2005	FY 2006	FY 2007
12.3	14.5	16.0 ^(a)	16.5 ^(b)	17.5 ^(b)	18.0 ^(b)	18.5	18.5 ^(b)
(a) Estimated. (b) Proposed.							

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