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

<table>
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<tr>
<th>Science Focuses</th>
<th>DOE Programs</th>
<th>B &amp; R Codes</th>
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<tr>
<td>Biology and Biogeochemistry</td>
<td>Engineering and Geosciences; Energy Biosciences;</td>
<td>KC-04, KC-06,</td>
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<td>Life Sciences; Environmental Remediation</td>
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<td>Materials and Chemical Sciences</td>
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<tr>
<td>Computational Sciences</td>
<td>Mathematical, Information, and Computational</td>
<td>KJ-01</td>
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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

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.
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 computations 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.
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.

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.
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,
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.

“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.”
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.

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
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.
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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

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• 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
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
Institutional Plan FY 2003-2007

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

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 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.
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 magneto-telluric 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.
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.

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

- **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.
• 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.

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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...
Institutional Plan FY 2003-2007

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 Chornobyl 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
Institutional Plan FY 2003-2007

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.

**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 providing science and technology knowledge and expertise in support of a new National Bureau of Asian Research initiative titled Tracking the Strategic Environment in Asia.
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
Institutional Plan FY 2003-2007

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.

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
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.
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.