

Appendix E
Laboratory Directed
Research and Development:
Renewing the Capabilities
at PNNL



Appendix E: Laboratory Directed Research and Development (LDRD): Renewing the Capabilities at PNNL

The LDRD program is the principal mechanism for renewing capabilities within the Laboratory and bringing forward novel ideas that will become the next generation of science and technology.

LDRD Program Benefits to DOE and the Laboratory

The LDRD program increases the value that PNNL provides to DOE as a multiprogram national laboratory. Many of the Laboratory's best scientific ideas were developed with LDRD funds and are now contributing to major DOE programs. They include the capabilities and instruments in our Environmental Molecular Sciences Laboratory, high-performance computational software tools that support a broad range of scientific simulations, climate change models, and technologies for immobilizing contaminants in soils and groundwater. Among the most promising new technologies developed under the LDRD program are high-throughput mass spectrometry, advanced microscopic imaging, and cell signaling and protein analyses capabilities that will help DOE and the broader scientific community better understand complex biological systems.

Today, the LDRD program supports the Laboratory in strengthening its base of scientific capabilities. As a multiprogram laboratory serving the challenging requirements of DOE's research and development focus areas, the flexibility provided by the LDRD program allows us to make rapid decisions on projects that address emerging scientific challenges facing DOE missions and to ensure that PNNL remains a modern research facility well into the 21st century.

Institutional Areas of Emphasis

The LDRD program supports new and innovative projects in each of the four research directorates at the Laboratory—Fundamental Science, Environmental Technology, Energy Sciences and Technology, and National Security. Projects cross organizational boundaries and link staff with similar expertise and research interests.

In line with our vision, the following major thrust areas for FY2004 are highlighted below:

Systems Biology and Biotechnology— Enhancing our systems biology and biotechnology capabilities is key to being at the forefront of scientific discovery in life sciences. In particular, the intersection with physics, chemistry, mathematics, and computational science and engineering provides a strong foundation for effective systems biology and biotechnology research. The Laboratory's LDRD projects in this area focus on enhancing fundamental systems biology and applied biotechnology capabilities, particularly as they apply to DOE's Genomes to Life program and the rapidly developing needs in bio-based products.

Computational Science and Engineering— Accomplishment of the Laboratory’s ambitious science and technology agenda requires a significant capability in the area of computational science and engineering. We are funding LDRD projects that are building and enhancing our capabilities in areas of computational science, mathematics, and engineering. The goal is to maintain a high-performance computing environment that supports PNNL’s key research areas, including atmospheric chemistry and transport, complex biological processes, subsurface science, and materials engineering and simulations.

Nanoscience and Nanotechnology— In addition to building a strong systems biology and biotechnology program, we want to establish a leading presence in nanoscience and nanotechnology with specific emphasis on nano-catalysis and nanobiology. The promise of nanoscience is the ability to design function at the molecular level, and then “teach” those molecules to self-assemble into more complex structures that can interface with biological systems or the macroscopic world. The Laboratory’s capabilities in self-assembly, thin-film deposition, oxide synthesis, and molecular modeling will be combined to generate a unique and world-class capability in this revolutionary area of science.

Nonproliferation and Homeland Defense— A number of our LDRD research projects support both Secretary Abraham’s emphasis on nonproliferation and homeland defense, and the needs of other federal agencies with interests and responsibilities in this area, such as the U.S. Department of Defense. Our efforts in imaging science and technology are focused on developing next-generation capabilities in image analysis and visualization, which ultimately will be beneficial to a diverse range of disciplines including counterterrorism, nonproliferation of weapons of mass destruction, and materials characterization.

Clean, Secure, and Affordable Energy—We are investigating heterogeneous catalysis, the exploitation of eukaryotic organisms in fermentation and enzyme discovery, and the development of novel reactor and separation systems that will enable us to resolve barriers that currently preclude successful and cost-efficient conversion of biomass into energy and high-value industrial products.

Environmental Quality— In the area of environmental quality, we are conducting research in process science and technology, which is directed toward characterizing materials, improving chemical processes, and identifying new technologies for waste management in ways that increase efficiency, reduce pollution, and perform novel functions. The focus of our efforts is on extending fundamental scientific developments in chemistry and materials to new microscale and conventional-scale systems. The results of this effort can be applied to waste management, environmental cleanup, and carbon management as it affects global climate changes, bio-based products, and processes for energy-intensive industries.

The *LDRD Program* at PNNL is an important mechanism for ensuring the future strength of our research and technology development capabilities. The program supports investigation of high-risk, high-value ideas. These capabilities and new ideas help the Laboratory to attract the best and brightest scientific staff needed to serve the highest priority DOE mission objectives. It is our principal means for supporting exploratory concepts, innovative approaches, and advanced studies needed to solve the most challenging scientific problems.

Effective Management of PNNL's LDRD Program

The effectiveness of PNNL's LDRD program management process is evident by the historical success of its projects. We continue to implement management measures in response to DOE and regulatory requirements.

Schedule

The major sequential steps governing PNNL's LDRD management process include the following:

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| May | The Director of Strategic Planning issues a formal schedule for research proposals, proposal review, and project reporting. Guidance for this process is prepared and issued annually. |
| May-June | LDRD proposals are solicited from research staff and selected projects are forwarded to Strategic Planning as candidates for potential funding. |
| July | The LDRD Program Office prepares and submits an annual LDRD Program Plan to DOE. |
| July-August | The Laboratory reviews LDRD project proposals using both internal staff and external experts. |
| September | Recommendations are forwarded to the Research Council for approval. |
| October | Principal investigators submit approved LDRD project proposals to the LDRD Program Office for review of compliance with DOE requirements. |
| October | The LDRD office forwards all projects to DOE-AMT for their review and signature for compliance with the DOE Order. |

The Laboratory's *Guide to Laboratory Directed Research and Development* is a brochure that provides guidance to Laboratory staff and defines the requirements of DOE Order 413.2A. This guide, available on the LDRD internal home page, describes accountability and reporting requirements for LDRD projects and the proper use of LDRD funds. The LDRD Program Office conducts reviews to ensure compliance with these criteria.

Plan

The LDRD Office at PNNL prepares and submits an LDRD Plan to DOE Headquarters that identifies the goals of PNNL's LDRD program, the broad scientific and technical areas planned for support, the maximum requested funding level, and any requests for fourth-year funding of specific projects.

Peer Review and Self Assessment

PNNL uses peer review to evaluate the quality, relevance, and performance of our scientific research. Peer review is the universally accepted process for determining the direction of and setting standards for scientific, engineering, and technology research and development. The Laboratory has a formal LDRD peer review process that ensures the technical integrity of our work, enhances our stature within the scientific community, and ensures that our research meets our customers' needs.

Research quality and the potential for research that leads to important scientific developments are best evaluated by employing respected subject matter experts and professionals. The Laboratory uses external peer review panels and conducts an analysis of technical accomplishments as judged by tangible output metrics for LDRD projects. In assessing the performance of LDRD projects, the following criteria are used: technical significance, technical approach, innovation, staff, technical environment, and technical progress. In addition, projects are evaluated to ensure they meet DOE missions and needs. Our review process includes using Advisory Committees, external reviewers for LDRD projects, and Directorate Review Committees.

In addition to technical peer review, the LDRD Program Office reviews projects for compliance with DOE Order 413.2A. Midyear and annual summaries of project performance are analyzed and linked to Laboratory critical outcomes. Project costs and spending rates are tracked in the Laboratory's financial system. Annual progress reports are obtained from the principal investigators for annual reporting, and tangible output metrics are obtained annually from each principal investigator and analyzed.

Laboratory Directed Research and Development Funding (Budget Authorization Dollar Amount in Millions)						
2002	2003	2004	2005	2006	2007	2008
15.5	7.9	18.5 ^(a)	19.0 ^(a)	19.5 ^(b)	20.0 ^(b)	20.0 ^(b)
(a) Estimated						
(b) Proposed						