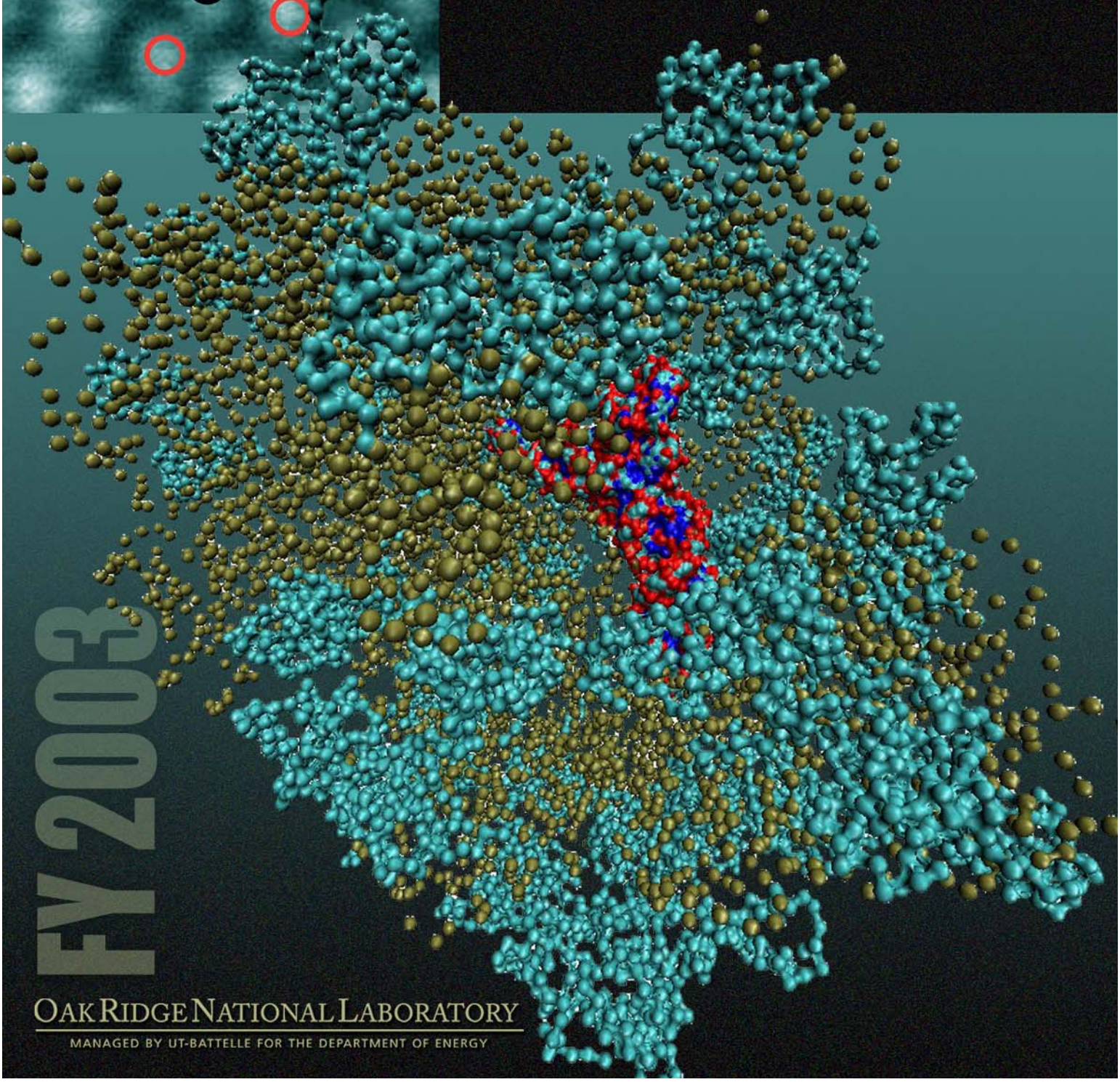
LDRD Annual Report

Laboratory Directed Research and Development



FY2003

OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

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Oak Ridge National Laboratory

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

FY 2003 ANNUAL REPORT

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INTRODUCTION

The Oak Ridge National Laboratory (ORNL) Laboratory Directed Research and Development (LDRD) Program reports its status to the U.S. Department of Energy (DOE) in March of each year. The program operates under the authority of DOE Order 413.2A, "Laboratory Directed Research and Development" (January 8, 2001), which establishes DOE's requirements for the program while providing the Laboratory Director broad flexibility for program implementation. LDRD funds are obtained through a charge to all Laboratory programs.

This report describes all ORNL LDRD research activities supported during fiscal year (FY) 2003 and includes final reports for projects completed during the year and shorter progress reports for projects that were active, but not completed, during this period. The *FY 2003 ORNL LDRD Self-Assessment* (ORNL/PPA-2004/3) provides financial data about the FY 2003 projects and an internal evaluation of the program's management process. It also contains information about new projects started during the first five months of FY 2004.

ORNL is a DOE multiprogram science, technology, and energy laboratory with distinctive capabilities in materials science and engineering, neutron science and technology, energy production and end-use technologies, biological and environmental science, and scientific computing. With these capabilities ORNL conducts basic and applied research and development (R&D) to support DOE's overarching national security mission, which encompasses science, energy resources, environmental quality, and national nuclear security. As a national resource, the Laboratory also applies its capabilities and skills to the specific needs of other federal agencies and customers through the DOE Work For Others (WFO) program. Information about the Laboratory and its programs is available on the Internet at <http://www.ornl.gov/>.

LDRD is a relatively small but vital DOE program at the Laboratory that allows ORNL, as well as other multiprogram DOE laboratories, to select a limited number of R&D projects for the purpose of

- maintaining the scientific and technical vitality of the Laboratory,
- enhancing the Laboratory's ability to address future DOE missions,
- fostering creativity and stimulating exploration of forefront science and technology,
- serving as a proving ground for new research, and
- supporting high-risk, potentially high-value R&D.

Through LDRD the Laboratory is able to improve its distinctive capabilities and enhance its ability to conduct cutting-edge R&D for its DOE and WFO sponsors.

To meet the LDRD objectives and fulfill the particular needs of the Laboratory, ORNL has established a program with two components: the Director's R&D Fund and the Seed Money Fund. As outlined in Table 1, these two funds are complementary. The Director's R&D Fund develops new capabilities in support of the Laboratory initiatives, while the Seed Money Fund is open to all innovative ideas that have the potential for enhancing the Laboratory's core scientific and technical competencies. Provision for multiple routes of access to ORNL LDRD funds maximizes the likelihood that novel and seminal ideas with scientific and technological merit will be recognized and supported.

The ORNL LDRD program recognizes that the R&D staff generally initiate new ideas, that peer review of proposals is an essential component, and that management has a role in fostering projects that are aligned with the strategic directions of the Laboratory. All proposals to the ORNL LDRD program undergo a rigorous review including peer review and must be approved by the Deputy Director for Science and Technology and concurred upon by DOE before funding can be provided.

Table 1. ORNL LDRD Program

	Seed Money Fund	Director's R&D Fund
Purpose	Supports core competencies	Supports laboratory initiatives
Year established	1974	1983
Funding cycle	Continuous	Annual
Proposal review	Proposal review committee	Initiative review committees
Project budget	≤$125,000	≤$800,000
Project duration	12 to 18 months	24 to 36 months
LDRD outlay	22%	78%

Director's R&D Fund

The Director's R&D Fund is the strategic component of the ORNL LDRD program and the key tool for addressing the R&D needs of the Laboratory initiatives. The initiatives, which are the focus of the strategic plan developed by ORNL in collaboration with DOE, are the critical areas that the Laboratory must concentrate on if it is to be prepared to meet future national requirements for science and technology.

The review and selection of Director's R&D Fund proposals is an annual process. In April, a call for proposals is issued to the research staff by the Deputy Director for

Science and Technology. In the call, ORNL's senior R&D managers identify specific research thrust areas that are critical to accomplishing the Laboratory's major initiatives. A committee is established for each thrust area to review the proposals and ongoing projects associated with that area.

The Director's R&D Fund has two rounds of review. In the first round, preliminary proposals are submitted to the appropriate review committee, which evaluates the ideas and selects a subset for development into full proposals. In the second round, each full proposal is peer reviewed for technical merit by two subject matter experts and presented to the review committee during the oral presentation sessions. Ongoing projects for which second- or third-year funding is being requested are also reviewed at this time. Following the presentations, each committee develops a funding recommendation for the suite of new proposals and ongoing projects in its charge. The Deputy Director for Science and Technology then reviews the committee recommendations, develops an overall funding strategy, and presents it for approval to the Leadership Team, ORNL's executive committee headed by the Laboratory Director. Based on the Deputy Director's recommendation, about 10% of the fund's annual allocation is usually held in reserve to support research projects of new R&D staff members who are being recruited to address strategic Laboratory needs.

In FY 2003, $12.5 million was allocated to the Director's R&D Fund to support 54 projects, 21 of which were new starts (see Table 2). Projects may continue for a maximum of 3 years, although most have a duration of 2 years.

Table 2. FY 2002 ORNL LDRD Breakdown by Fund

	Seed Money Fund	Director's R&D Fund
Costs	$3.56 million	$12.5 million
Number of projects	69	54
Number of new starts	40	21
Number of continuing projects	29	33
Average total project budget	~$89,000	~$488,000
Average project duration	15 months	25 months

Director's R&D Fund Research Thrust Areas

In requesting proposals for FY 2003, the Laboratory's senior R&D managers developed thrust areas to support the research needs of the Laboratory initiatives in advanced materials, complex biological systems, energy and environmental systems of the future, national security, neutron sciences, and terascale computing and simulation science. These thrust areas are briefly described below. Detailed descriptions of the Laboratory initiatives and the LDRD research thrust areas are provided in the *ORNL Institutional Plan FY 2003–FY 2007* (ORNL/PPA-2002/2). The levels of investment in the thrust areas are summarized in Fig. 1; an index of projects by initiative is provided on p. 433.

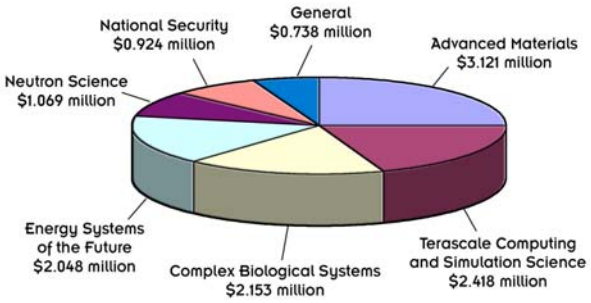

Fig. 1. Level of Director's R&D Fund investment in the Laboratory-wide initiatives for FY 2003.

Advanced Materials

The focus of the advanced materials research thrust is nanoscale science, engineering, and technology, an area that is expected to provide breakthrough opportunities in many fields central to DOE's missions, including materials science, biotechnology, processing science, energy, environmental technology, information technology, and national security. A high priority was given to the development of capabilities for the controlled synthesis of nanomaterials and nanostructures, resulting in functionality for nanoscale systems.

Complex Biological Systems

The research thrust in complex biological systems builds on ORNL's expertise in the life and environmental sciences, chemical and analytical sciences, instrumentation sciences, and computational sciences. In FY 2003, this thrust aimed at the development of new molecular and computational capabilities and approaches in response to DOE's proposed Genomes to Life Program and genomics tools and computational strategies to further our understanding of the natural and pathological functioning of cells from microbes to higher organisms (humans, mouse, fish, plants, etc.).

Energy and Environmental Systems of the Future

This research thrust area seeks to build new R&D capabilities that promote the development of new energy services that are environmentally responsible and economically competitive. It is focused on meeting the increasing demand for energy throughout the world while

recognizing that a very large proportion of today's energy needs are met through resources and technology systems that are nonsustainable. Thus, ways to increase the availability of energy, safely and affordably, while shifting to significantly different energy paths with minimal effects on human health and the environment will be required. Making this shift will require a thorough understanding of a broad range of science, technology, economic, and policy issues that will drive the development of future energy systems.

National Security

As a DOE multiprogram laboratory, ORNL possesses critical capabilities that can provide federal and state authorities with the technologies and expertise required to protect the public. The objective of this thrust was to develop leading-edge capabilities to increase national security. In FY 2003 this thrust addressed (1) sensors and detectors for chemical, biological, and nuclear threats; (2) computer and computational science for homeland security; and (3) transportation security.

Neutron Sciences

The Spallation Neutron Source (SNS) and the upgrades at the High Flux Isotope Reactor (HFIR) that will be completed as part of the Laboratory initiative in neutron sciences offer a unique opportunity for ORNL and the nation to demonstrate world leadership in this area. The success of these projects (and their impact on ORNL) depends critically on the ability to develop the full potential of these new scientific tools and to integrate neutron sciences into research programs across the Laboratory. The intent of this research thrust area is to stimulate new research directions, proof-of-principle experiments, and technical innovations essential to achieving leadership in neutron science. This thrust area focuses on three research themes that are essential to leadership in neutron sciences: novel applications of neutron scattering, neutron physics, and novel instrumentation concepts.

Terascale Computing and Simulation Science

This research thrust recognizes that new computational tools and codes are needed to enable the creation of realistic simulations of physical situations and to provide new insights into a host of scientific problems. Research, development, and deployment of mathematical models, computational methods, numerical libraries, and scientific codes are needed to take full advantage of the capabilities of ORNL's terascale computers for solving strategic or critical problems in materials sciences, chemistry, combustion, accelerator design, high-energy physics, nuclear physics, fusion, biology, and global systems.

Seed Money Fund

The Seed Money Fund complements the Director's R&D Fund by providing a source of funds for innovative ideas that have the potential of enhancing the Laboratory's core scientific and technical competencies. It also provides a path for funding new approaches that fall within the distinctive capabilities of ORNL but outside the more focused research thrusts of the major Laboratory initiatives. Successful Seed Money Fund projects are expected to generate new DOE programmatic or Work-for-Others sponsorship at the Laboratory.

Proposals for Seed Money Fund support are accepted directly from the Laboratory's scientific and technical staff (with management concurrence) at any time of the year. Those requesting more than $20,000 ($125,000 is the maximum) are reviewed by the Proposal Review Committee (PRC), which is comprised of 11 scientific and technical staff members representing each of the Laboratory's research divisions and the LDRD manager (chair). To assist the Committee, each proposal is also peer reviewed by two Laboratory staff members selected by the LDRD manager. Proposals requesting $20,000 or less are not reviewed by the PRC but are peer reviewed by a research staff member selected by the LDRD manager. All Seed Money Fund proposals receiving a favorable recommendation are forwarded to the Deputy Director for Science and Technology for approval and require DOE concurrence.

In FY 2003, $3.6 million of the LDRD program was apportioned to the Seed Money Fund to support 69 projects of which 40 were new projects (see Table 2). The distribution of Seed Money Fund support by science and technology area is shown in Fig. 2. The assignment of projects to specific areas is not meant to be definitive as many projects are crosscutting and could be assigned to more than one category.

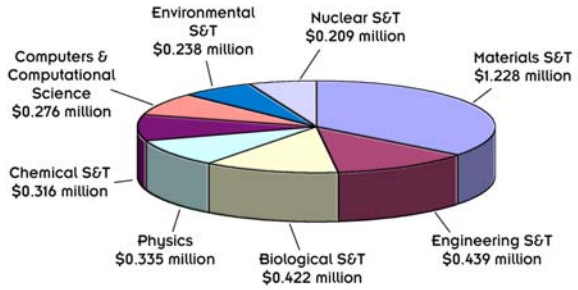

Fig. 2. Distribution of Seed Money by science and technology area for FY 2003.

Report Organization

The report is divided into eight broad areas of science and technology that underlie the programmatic and Work for Others activities at ORNL. Within each of these areas, the projects are grouped by fund (i.e., either the Director's R&D Fund or the Seed Money Fund). Within each fund grouping are the final reports and progress reports in that order. A list of Director's R&D Fund projects by initiative an author list, and a project list are included at the back of this document.