DOE Research and Development Portfolio

Science

Volume 4 of 4 / February 2000

U.S. Department of Energy

Department of Energy
Washington, DC 20585

February 2000

The Department of Energy's investments in Science are investments in America's future. The knowledge sought by our scientists address some of the most profound questions and daunting challenges facing humanity – challenges that both hold the keys to our long-term prosperity as a nation and feed our sense of exploration and discovery. Built around core competencies, basic research will continue to explore potentially new forms of clean energy, develop solutions to some of our more pervasive energy-related pollution problems, decode the mysteries of the human genome, reveal the secrets of matter and energy, and advance the state of simulation and computation. In short, our programs will expand the frontiers of basic research and the instruments of science that are the foundations for the Department's applied missions, the base for U.S. technology innovation, and the sources of remarkable insights into our physical and biological world.

The Department of Energy (DOE) has undertaken a major effort to ensure that our research and development (R&D) programs and Federal R&D investments are balanced, focused on mission, and appropriately coordinated with the needs of our clients, the public and the marketplace. To do this, we are instituting a new portfolio approach to managing our R&D activities. This entails building a comprehensive document that provides in one place, a clear description of our entire $7.6 billion research portfolio. This volume describes DOE's Science R&D Portfolio. It is Volume 4 of the DOE's four-volume R&D Portfolio. The full set in the series includes one R&D portfolio volume for each of DOE's four major business lines, plus an Overview.

The Science R&D Portfolio focuses on the FY 1999-2001 timeframe. Its purpose is to help (1) describe our current R&D activities and showcase recent accomplishments; (2) evaluate whether our portfolio is appropriately balanced to meet our long-term strategic mission goals; (3) align our R&D investments with broader national policy goals; and (4) plan for future investments through roadmapping.

The investments presented in the Science Portfolio are important and creative steps toward bringing forth the scientific knowledge, innovation, technologies, and partnerships required to meet the challenges of the next century. It is our hope that this document will provide the means for illuminating our proposed investments for Fiscal Year 2001 and beyond, as a unified portfolio, and serve as a useful framework and resource for further analysis and dialogue among all interested parties.

Ernest J. Moniz
Under Secretary

James F. Decker
Acting Director
Office of Science

Foreword

This report summarizes the Department of Energy's Science Portfolio. It reflects new thinking developed over the last two years on the way we approach, analyze, plan, and describe our science programs within a long-range strategic science framework. Informed by over one hundred of the nation's leading scientists, technologists, end-users, futurists, and planners during two national workshops, this portfolio has three goals:

- Connect science programs and activities with the fundamental questions that they address, and articulate the motivation and importance behind these questions.

- Illuminate and capitalize on the connections and opportunities at the boundaries of science disciplines, recognizing that now, and increasingly in the future, advancing the frontiers of science requires multidisciplinary approaches and capabilities.

- Define near-term, next steps on the path forward to tackling some of the major scientific challenges that lie ahead.

This Science Portfolio is part of a broader Departmental initiative outlined by the Under Secretary of Energy to review all of the research and development, basic and applied, within DOE. This is the first of a series of planned annual updates to our portfolio, a dynamic process built upon this new, long-term strategic science framework. We believe that this approach helps to lay a strong foundation for future planning, analysis and, ultimately, scientific discovery.

These past two years marked a critical step for DOE's science programs. Starting in January 1998, we launched several complementary efforts, one of which resulted in the initial portfolio description and analysis, and ultimately, this new version. This summary provides perspective on the role of this portfolio, in context of all the efforts toward a more integrated, fundamental look at future science opportunities and directions. Specific elements of this approach are as follows:

- ***Science Themes and Strategic Framework***—A national workshop and series of follow-on efforts, begun in early 1998 and completed by the end of the year, were designed to encourage national debate on long-term *themes* and *directions* of DOE's science portfolio. Participating in the debate were some of the nation's leading scientists, technologists, end-users, planners, and futurists.

- ***Strategic Plan***—Published in June 1999, the strategic plan articulates the strategic *goals, objectives,* specific *strategies* as well as *performance measures* for DOE's science program, extending out 20 years or more. It builds on the science themes and strategic framework.

- ***Science Portfolio—***A detailed description and summary analysis of DOE's current science investments, the portfolio identifies the *activities, accomplishments*, and *motivation* for the research, as well as the near-term *resources*. It too is built on the major science themes and strategic framework.

- ***Science Roadmaps***—The Office of Science launched efforts to perform detailed roadmaps in several areas of science investigation: complex systems, carbon sequestration, non-defense scientific supercomputing, and science facilities. Each is at a different stage of completion. Unlike either the Portfolio or the Science Strategic Plan, the roadmaps chart the *necessary steps* and *sequence* to achieving a desired end goal. This path includes considerable *detail* at the research and activity level, and relative to the Portfolio, extends over a longer time frame. *Contingencies* are built into the roadmap to ensure success and deal with technical and institutional uncertainties.

This report contains a summary section and detailed sections that correspond to major science challenges. These challenges flow from the strategic science framework developed earlier in the year. The summary section includes appropriate background and a portfolio discussion. The challenge sections include detailed information on the purpose, description, activities, and accomplishments for research aligned with that challenge.

Table of Contents

Executive Summary

National Context/Drivers.

Much has been written on the value of basic research and its profound effects on our nation's economic growth, quality of life, and security. This century has witnessed a great age of scientific discovery, and DOE's science programs have played a leading role. Scientists have learned to control matter at the atomic level, explored the origins and fate of the universe, established the basis for a complex and far-reaching energy system, and found ways to help protect and restore the environment. And as the pace of scientific discovery and technological advancement accelerates, new challenges in complexity will require interdisciplinary approaches and a more seamless, interconnected science establishment.

In recent years, a shift has occurred within industry toward research investments with shorter time-horizons and with greater near-term payoffs—shifts away from basic research. Consequently, government programs are under greater pressure than ever to advance the scientific knowledge-base that is essential to fuel future innovation. Science programs are being called upon to deliver more for less, and managers and scientists must scrutinize and prioritize investments more carefully than ever before. Science investments that solve problems in other segments of the economy (e.g., environmental cleanup) often save considerable resources that are then available for investment elsewhere in the economy, including further investments in science. In general, science investments are high leverage, with diverse implications not only for applied R&D and technology, but for other scientific investigations. Many of the accomplishments identified in this report tell discovery stories with far-reaching impacts.

DOE's science portfolio responds to the overall Departmental challenge articulated in the DOE Strategic Plan, that is, to:

> "Deliver the scientific understanding and technological innovations that are critical to the success of DOE's mission and the Nation's science base".

DOE/Federal Role

DOE is a science agency. The Department of Energy is the third largest government sponsor of basic research in the United States. Research programs and infrastructure supported by DOE, including the DOE national laboratory system, underpin the agency's applied missions in energy, environment, and national security. More generally, DOE's science programs and infrastructure extend the frontiers of fundamental research. DOE leads the nation in much of the physical sciences, and contributes in major ways to advances in biology and environmental science. Accelerators, light sources and neutron beam facilities, plasma and fusion science facilities, and genome and advanced computational centers are just some of the major instruments of science that distinguish the Department of Energy and substantially enhance the nation's science base.

Consistent with the goals of basic research, the purpose of DOE's science portfolio is to explore and extend our understanding of the complex phenomena and processes that define our physical world, to determine what factors influence them, and to understand how we may ultimately control them. Research activities span the continuum of science, ranging from fundamental investigations into the nature of matter and energy and the origins and evolution the universe, to strategic basic research that underpins and supports advances in applied technologies—technologies vital to DOE's mission, ranging from new systems for harnessing energy to improved methods for environmental cleanup.

Program Summary and Trends

With only minor exceptions, the science portfolio of the Department is contained within and managed by DOE's Office of Science. The Department of Energy is responsible not only for research in the basic sciences, but for maintaining the necessary infrastructure to conduct this research—the national laboratories, advanced instrumentation, computational abilities, the next generation of scientists, and supporting infrastructure. Beyond its own research programs, DOE operates many scientific facilities that provide open access to the nation's public and private sector scientists.

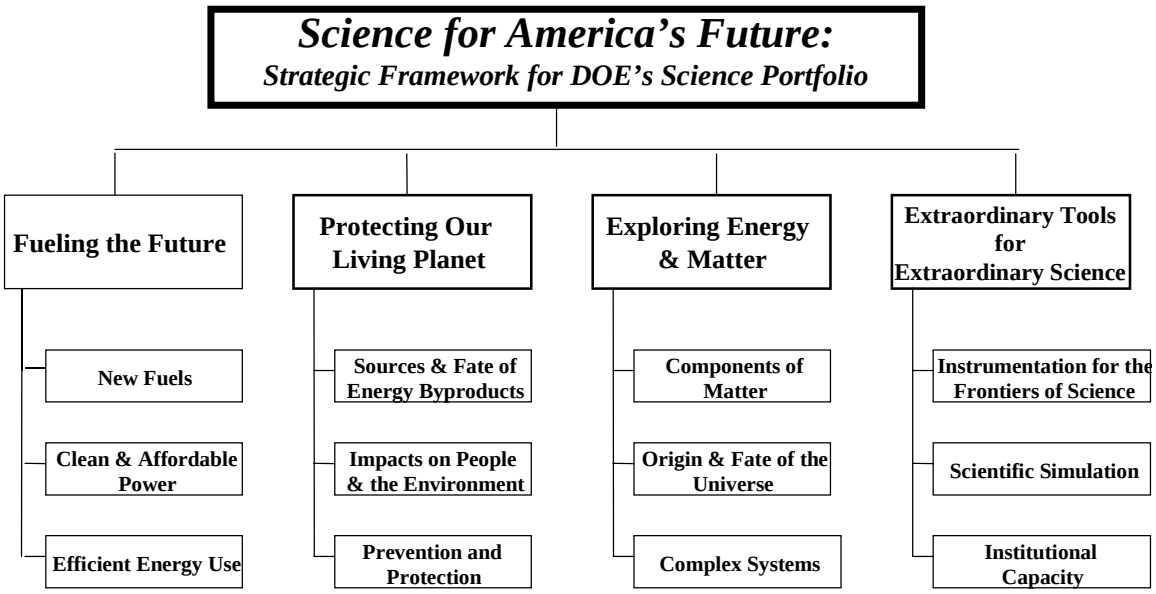
The actual research performed by DOE is carried out in DOE's national laboratories, colleges and universities, and industry. Roughly 72% of funding goes to the national labs, 23% to universities, and 5% to industry.

Recently, the Department organized its research and science activities around four major science themes, reflecting a crosscutting perspective on the science goals of the agency. These themes are:

- **Fueling the Future**—Science for affordable and clean energy.
- **Protecting Our Living Planet**—Energy impacts on people and the environment.
- **Exploring Matter and Energy**—Building blocks of atoms and life.
- **Extraordinary Tools for Extraordinary Science**—National assets for multidisciplinary research.

Within each of these areas, individual science challenges have been identified that further organize and illuminate the paths forward for the Department's basic research, as depicted below.

In its purest form, the long-term, high-risk research that is the natural domain of government is highly uncertain. Testing hypotheses and expanding the frontiers of knowledge is nothing less than a conscious effort to challenge uncertainties—the uncertainties of theories, the uncertainties of outcomes, the uncertainties of next steps, and, more basically, the uncertainties of exploration.



Guided by a rigorous advisory committee and peer review process that draws on the talents of internationally renowned scientists in their fields, the Department plans its long-range investments and makes constant adjustments in response to the discovery process.

Within the overall directions of research summarized in this science portfolio, there are some areas where emphasis and corresponding investment trends are changing. The motivations behind these changes are described in the body of this report.

Within the science theme of *Fueling the Future*, there is increased emphasis on the science that underpins carbon recycling and improved energy efficiency, simulation for combustion and materials, and fusion plasmas.

Under *Protecting Our Living Planet*, there is increased emphasis on science for carbon sequestration, human and microbial genomics, structural biology, radiopharmaceuticals and functional imaging, biomedical engineering, the health impacts of low dose radiation, environmental remediation, regional climate modeling/simulation, and advanced monitoring and sensors. De-emphasis is occurring in radioisotope development and high-dose radiation biology.

Within *Exploring Energy and Matter*, there is an increased emphasis on science for complex systems and the underlying interdisciplinary mix that will enable advances on this frontier, neutrino science as well as accelerator and non-accelerator based investigations into the nature of energy and matter and the origins and fate of the universe, university research in high energy and nuclear physics, international collaboration on large high energy physics facilities, plasma turbulence theory and experiments, understanding the complete workings of a microbial cell, and functional genomics and investigations of the properties and implications of organisms in

extreme environments. There is less emphasis on unilateral support for next generation high energy physics facilities.

Under *Extraordinary Tools for Extraordinary Science,* there is increased emphasis on advanced computation and associated hardware and software, imaging and visualization science and technology, scientific data management, upgrades to neutron science facilities and building the Spallation Neutron Source, collaboratories and interconnected science facilities, use of synchrotron radiation sources for research in the life sciences and structural biology, collaborations with the National Institutes of Health and the National Science Foundation and others on facility design and use, and science education. Also, there is continued emphasis on the international program to build the LHC—the world's highest energy proton collider, and research programs to exploit the recently completed B-Factory, Main Injector and RHIC in order to pursue extraordinary insights into the components of matter and the origin of the universe. De-emphasis is occurring in the continued support for outdated experimental facilities.

Aside from these general trends, there are new or notably expanded areas of science emphasis in FY 2001. Highlights of these are provided below.

- ***Nanoscale science***, engineering and technology research to understand how deliberate tailoring of materials can lead to new and enhanced functionality and to provide new experimental and computational modeling tools for nanoscale research. *(+$36 M).*

- ***Advanced scientific computing***, including computational modeling and simulation in broad areas of fundamental science *(+$51 M).*

- ***Bioengineering sciences***, capitalizing on unique instrumentation at DOE's national labs that enable the advancement of fundamental concepts in biologics, materials, processes, implants, devices and informatics systems for subsequent prevention, diagnosis, and treatment of disease *(+$5 M).*

- ***Microbial cell research*** aimed at understanding the complete workings of a microbial cell to help meet needs in many diverse research areas such as energy, bioremediation, and carbon sequestration *(+$12 M).*

- ***Climate Change Technology research***, a program addressing carbon management in areas of science for efficient technologies, fundamental science underpinning advances in low/no-carbon energy sources, and sequestration science *(+$4 M).*

- ***University-based research in robotics and intelligent machines*** for future applications important to DOE missions and to enable remote access to the DOE Office of Science user facilities *(+$2 M).*

- ***Construction of the $1.4 billion Spallation Neutron Source*** at Oak Ridge National Laboratory to regain the U.S. position of international leadership in neutron scattering for the physical, chemical, materials, polymer, and biological sciences *(+$163 M).*

- ***Support for scientific user facilities*** by providing funds to optimize operating time and user support to serve more than 15,000 scientists in academia, industry, and federal laboratories who use these facilities annually. *(+$68 M).*

Key Accomplishments

DOE's science programs have a long and rich history of remarkable discoveries leading to 70 Nobel Prizes awarded to scientists supported by DOE—a total that far surpasses that of any other public or private institution. As recently as December of 1998, DOE research at the Lawrence Berkeley National Laboratory was awarded Discovery of the Year by the journal *Science*. The Berkeley scientists discovered, through innovative experiments looking at supernovas and redshift, that the universe seems to be expanding at an accelerating rate, suggesting a strange and yet-to-be explained property of space. Also recently, DOE completed the genomic sequencing of a microbe, Deinococcus radiodurans – dubbed Conan the bacterium by the press, that can survive incredible doses of radiation and has been modified in laboratory experiments to clean-up solvents and metals found at DOE waste sites. DOE's Joint Genome Institute also contributed to the completion of a draft sequence of the entire human genome scheduled for completion in the spring of 2000, by completing the sequence of human chromosomes 5, 16, and 19. In a final example, DOE scientists exceeded 1 teraflop in sustained computational performance in an application.