DOE Research and Development Portfolio

Science

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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.

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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.

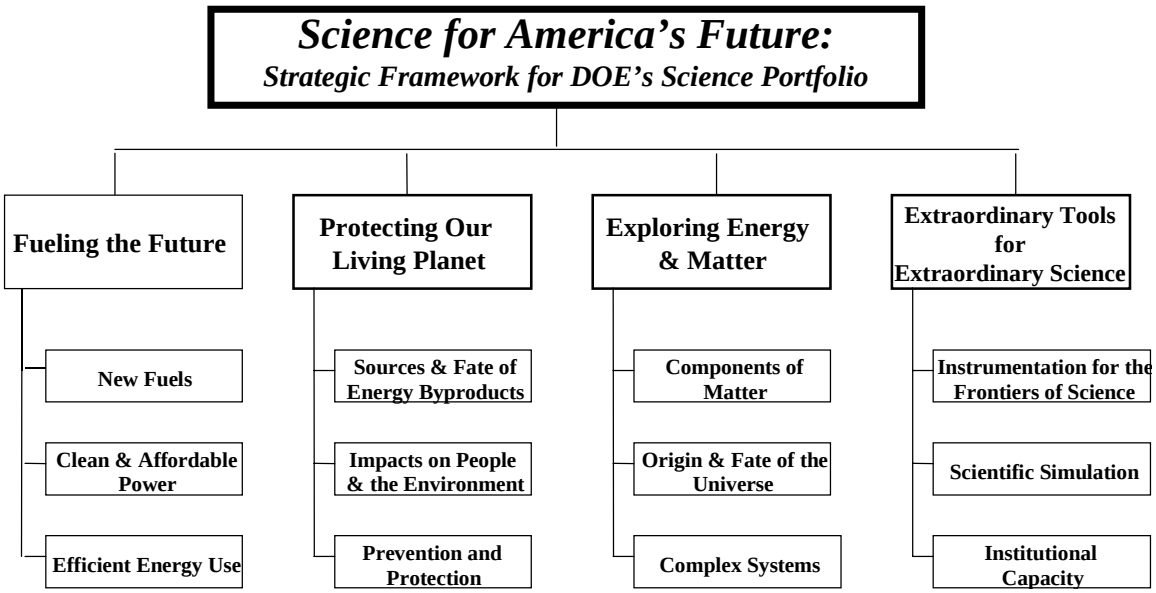
The actual research performed by DOE is carried out in DOE's national laboratories, colleges and universities, and industry. Roughly 72% of funding goes to the national labs, 23% to universities, and 5% to industry.

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.

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Introduction

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Overview

The fact that the United States enjoys a high standard of living and a prosperous economy is partly attributable to our willingness as a nation to invest significant public resources for public goods not readily attainable by the normal workings of the marketplace. Much has been written on the value of basic research and the role of the federal government in sponsoring such research. The National Academy of Sciences, articulating a widely held view, notes that much of this nation's economic growth, quality of life, and security derive from previous investments and our national ability to lead in science and technology. The Department of Energy directs a sizeable portfolio of basic science that underpins DOE's applied R&D missions and that explores broad frontiers in fundamental science, leading the nation in the basic energy sciences and much of the physical sciences, and contributing to major advances in biological research.

Leading nations throughout the world sponsor basic research. The United States has historically held a leadership position in government-sponsored research. More and more, however, the complexity and the expense of basic research are increasing, and the private-sector finds such research increasingly difficult to support, especially when faced with near-term financial objectives. This shift by industry away from long-term, basic research toward applied research and development has been well documented in recent years and has created a sizeable vacuum for government-sponsored research to fill. The substantial benefits to the nation and indeed the long-term prosperity of the country depend on these investments. The benefits are real, as are the problems and challenges that they address. For example, major scientific discoveries at DOE are creating remarkable new opportunities and are leading the way toward radically new technologies, solutions to energy and environmental problems, and entire spinoff industries in such areas as:

- Hydrogen-based energy systems.
- High-temperature superconducting wires and devices.
- Batteries thinner than plastic wrap.
- Teraflop computers that set world benchmarks for speed.
- Medical diagnosis and imaging technologies.
- Biomolecular design based on DNA sequencing.
- Ion beam and plasma technology.

The energy and environmental problems of the future will likely be more complex and harder to deal with than those faced to date. Meeting the challenges of the future will often require entirely new approaches and options—revolutionary, not just evolutionary changes in technology. The key to this ability rests on advancements in basic science.

DOE—A Science Agency

With only minor exceptions, the Science Portfolio of the Department is contained entirely within DOE's Office of Science (SC). Formerly the Office of Energy Research, this office was given a new name by Congress during the FY 1999 budget deliberations, in recognition of the broad science mission of DOE and more than 50 years of contributions to basic research.

Top Five Government Research Organizations for Basic Research*

1. Health and Human Services ($8.0 B)
2. National Science Foundation ($2.5 B)
3. **Department of Energy ($2.5 B)**
4. NASA ($2.1 B)
5. Department of Defense ($1.1 B)

* Numbers are from FY 99 President's Request in Billions and include adjustments to enable comparisons. Source: OMB.

Overall, DOE's science portfolio totaled almost $2.7 billion in FY 00, and the data available for FY98 indicate that at that time, DOE was the third largest supporter of basic research in the United States.

Nearly **$2.7 billion** went into direct support for basic science, research facilities, and related infrastructure in FY 00. The budget, traditionally laid out by general science *discipline*, is depicted in the table below.

DOE's Science Portfolio Budget ($ Millions)*

	FY 99	FY 00	FY01
Basic Energy Sciences	759	720	963
Biological & Environmental Research	428	435	445
High Energy Physics	664	669	685
Nuclear Physics	321	330	350
Fusion Energy Sciences	216	238	240
Advanced Scientific Computing Research	153	125	175
Total All Other Science R&D Portfolio	154	144	157
Totals**	2695	2660	3015

*Excludes Program Direction
**Totals reflect accurate summation of numbers above, each carried to significant figures not shown.

Research in these disciplines is actually carried out at the national laboratories, universities and colleges, and at private-sector institutions under the direction and guidance of the Department.

A History of Discovery – The Promise of Discovery

This century has been a great age of scientific discovery, and DOE's science programs and national laboratories 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 the pace of scientific discovery and technological advancement is accelerating dramatically.

For example, within just the last few years, DOE scientists have discovered a chemical responsible for cell-to-cell communication and have identified archeabacteria, which represent a third kingdom of life. The discovery of a new electrolyte system (lithium phosphorus oxynitride) has enabled the development of thin-film batteries with unsurpassed energy densities and the ability to operate safely at temperatures as high as 150 degrees Centigrade. A newly designed, elegantly simple experiment allows scientists to examine the interaction of chemistry and turbulence in quantifiable and verifiable detail for the first time. Light bulbs, fluorescent tubes, and neon lights may soon become things of the past, replaced by more efficient and brighter lighting sources utilizing light-emitting diodes (LEDs) based on newly improved gallium nitride semiconductors. A new field of optics came into being, based on a new way to capture and focus light. Scientists have introduced a set of solvent-degrading genes from one microbe into a radiation- and desiccation-resistant bacterium, thus demonstrating the potential for designing microbes that could survive in high-radiation environments and degrade or detoxify other contaminants. Research has confirmed that biogenic hydrocarbon chemistry is key to understanding ozone and other oxidant production in the eastern United States A new

DOE Science—Some Recent Breakthroughs

- Discovery of the Year (in the journal *Science*) that the universe seems to be expanding at an accelerating rate, based on research into supernovas and redshift.
- Genomic sequencing that confirmed a new, third kingdom of life on Earth that includes a deep ocean, methane-producing organism.
- World record for sustained fusion reaction in both length of reaction and peak energy.
- Discovery of the top quark, the last, unusually large subatomic element that helps flesh out the Standard Model.
- Calculation of Black Hole entropy from super-string theories.
- Improved high temperature superconductors through research into pairing mechanisms and vortex physics.
- Potential new ways to store hydrogen through the discovery of new graphite nanofibers that can store three times their weight of hydrogen.
- Computational ability that recently exceeded 1 teraflop in sustained performance for an application.
- Artificial photosynthesis through research into light-matter interactions and solar photochemistry.
- Collaboration in the development of a photovoltaic cell that holds three world records for efficiency.
- Improved miniaturization through research into nanowires: "magic structures" and conductance quantization.
- Improved models and measurement of the carbon cycle, the phenomenon of global warming, and the role of cloud formation.
- A tenfold increase in the electrical conductivity of semiconductors through research into gallium injection.
- Development of the current generation of high energy, power lithium and lithium ion batteries from research into non-aqueous electrolytes.
- Development of treatments for diseases and addictions that are newly enabled by PET brain imaging studies.

generation of observing tools and instruments are now making ground- and atmosphere-based measurements of clouds and atmospheric radiation.

DOE researchers sequenced more than 300 million base pairs of draft and high quality human DNA sequence, and genomic DNA sequencing has been completed on microbes related to bioremediation and carbon sequestration. Positron emission tomography (PET) and magnetic resonance imaging (MRI) have been merged, opening new possibilities in diagnostic imaging. Scientists have discovered elementary particles and their interactions. The development of super-string theory is a major step on the road to a unified theory of forces.

In support of its science programs, the Department manages the most extensive and advanced complex of scientific facilities in the world. Such facilities include powerful accelerators for high energy and nuclear physics, light and neutron beam facilities for the natural and life sciences, electron beam microcharacterization centers, multidisciplinary mission centers, and single-purpose research facilities. Through its computing facilities, the Department is enabling rapid strides in scientific simulation as an equal partner to laboratory science in testing concepts and modeling complex processes.

DOE's science programs have a long and rich history of remarkable discoveries. To date, 70 Nobel prizes have been awarded to scientists supported by DOE—a total that far surpasses that of any other public or private institution. It is not surprising then that the future can be viewed with such great optimism.

Themes and Challenges at the Frontiers of Science

Over the past year, DOE has prepared a strategic framework to enhance its long-term thinking—a framework that reveals new opportunities at the boundaries of science disciplines, and one that identifies the major science ***themes*** and corresponding science ***challenges*** that, in keeping with our mission, define our purpose and guide our long-term actions. The four major themes for science are (1) Fueling the Future, (2) Protecting Our Living Planet, (3) Exploring Matter and Energy, and (4) Extraordinary Tools for Extraordinary Science. These themes, and corresponding challenges, are outlined below.

Fueling the Future
— Science for affordable and clean energy

Providing scientific foundations that keep the United States in a leadership position for abundant, affordable and clean energy is essential for a strong and secure nation. Fueling the Future is a critical theme, for it addresses the scientific foundations for the Department's applied energy technology programs. The future of U.S. energy systems relies on basic research that allows existing energy systems to become cleaner, safer and more efficient—and, just as important, understanding what new fuels can be created and harnessed.

What new energy sources can be created and harnessed? American security and welfare require sustained, abundant, and clean energy. The Science Portfolio is addressing the demand for energy by providing the scientific foundation for energy production from carbon-free or low-carbon sources. Research on hydrogen-based energy systems and other carbon-free energy supplies is critical to this need. Central to meeting the long-term demand for energy is research on the science of controlling plasmas for fusion to understand fusion confinement systems and the properties of plasma ignition and behavior. Bioenergy systems, including improving photo-synthetic systems and energy conversion systems, are central to this problem. Energy research is also developing the detection instrumentation, monitoring, and modeling systems to understand the behavior of the earth's interior to better tap geothermal and petroleum energy supplies.

How can energy systems be made cleaner, safer and more efficient? Improvement in the efficiency, safety and cleanliness of energy technologies requires better materials and better conversion and utilization processes. At the heart of these challenges are advanced materials and high performance structures that can withstand demanding environments, including high temperature materials for more efficient combustion systems or high performance structures that may be tough, low friction or high strength. Improved catalysis and conversion processes can realize significant improvements in combustion and exhaust gas cleanup systems and improve yield of fuels and valuable chemicals in photoconversion. Developments in quantum engineering hold the promise of widespread deployment of high temperature superconducting materials, advanced electronic materials, or other materials with advanced properties from molecular design and assembly.

Fueling the Future poses the following major *scientific challenges* for DOE's science portfolio.

Challenges

- ***New Fuels***—To understand the geological, chemical, biological, and physical processes for clean and affordable domestic fuels.

- ***Clean and Affordable Power***—To understand the physical, material, and chemical processes for advanced power generation, storage and transmission.

- ***Efficient Energy Use***—To understand the engineering, materials, and chemical processes to develop new energy efficient technologies.

Protecting Our Living Planet
— Energy Impacts on People and the Environment

As world population and the energy intensity of society increases, our planet is beset by increasing pollutants and waste streams. It is increasingly critical that we understand the complex interactions between man-made energy-related pollutants and the environment and living systems. Only through this understanding can effective strategies for mitigating the effects be developed. Protecting Our Living Planet is the theme that embraces these important science issues. Some of the key questions include:

What are the sources and fate of energy-related pollutants? Understanding the genesis, transformation, transport, and concentration of energy-related pollutants is the key to predicting their local, regional, and global effects. Advanced sensors and monitoring, with improved modeling and simulation, are required to understand these complex phenomena. This information is crucial for the information base that supports policy and regulatory decisions on energy and environmental matters.

How do complex biological and environmental systems respond to our energy use? Steeped in a long tradition of research aimed at understanding the biological effects of radiation, DOE-supported researchers have developed and applied some of the most advanced and sensitive analytic techniques to the examination of energy-related pollutants and their interaction with biological systems at the molecular, cellular, and organism levels. Similarly, DOE support has led to the development of information and models that can be used to explore the complex effects of pollutants on ecological systems at local and global scales. Additional basic research will reveal new and improved ways of protecting and restoring the environment, including the use of bioengineered micro-organisms for the restoration of contaminated land and water.

What factors change global climate and how can they be controlled? Perhaps one of the most pressing global environmental/energy issues of our time is the emergence of global climate change. Research in understanding the phenomenon, the rate of change, and ways to manage the carbon cycle more effectively will offer the long-term solutions that will shape our energy future.

Protecting Our Living Planet presents the following major *scientific challenges* for DOE's science portfolio:

Challenges

- ***Sources & Fate of Energy Byproducts***—To understand the molecular, atmospheric, geological, and biological pathways of energy byproducts in the biosphere.
- ***Impacts on People and the Environment***—To understand and evaluate the effects of energy byproducts on people and the environment.
- ***Prevention and Protection***—To create new scientific approaches to protect the biosphere from the effects of energy byproducts.

Exploring Matter and Energy
— Building Blocks of Atoms and Life

Understanding the nature of matter and energy and how these interact to form the material world presses the bounds of human imagination, mathematics, computation, and instrumentation. To understand the nature of matter and energy at the most fundamental level is an important science theme for DOE and one where it has traditionally held a worldwide leadership position. The key questions to be addressed through this exploration include the following:

What are the fundamental building blocks of matter? Understanding the nature of matter requires that the origin of mass of the most fundamental particles be determined, including the underlying constituents. The properties of quarks must also be understood, as well as the structure of nuclear matter, exotic high energy nuclei and matter under normal temperatures and pressures on Earth. The standard model explains the properties of matter that must be understood, including explanation of observed violations of the standard model, such as parity non-conservation. An extensive experimental program using high energy and high luminosity colliding beam accelerators is needed to explore the building blocks of matter as well as many other experiments designed to shed light on the standard model and to help bring together all of the known strong and weak forces into a unified theory.

How can the origin and fate of the Universe reveal the secrets of matter and energy? At the birth of the Universe, following the Big Bang, energy began to condense into quark-gluon matter, and into nuclear matter. The Universe is now expanding at a great rate, and understanding the conditions of the early universe and the fate of the expansion can reveal the secrets of the form of matter and energy. This question addresses why the universe is dominated by normal "matter" rather than "antimatter," an asymmetry of matter that is a major enigma. The fundamental forces and properties of matter are incompletely characterized, so that a coherent, unified concept of the forces is needed.

How do atoms and molecules combine to form complex dynamic systems? Understanding the origins and structure of the material world is essential to harness energy, develop new materials, and improve the quality of life. For example, the behavior of extremely hot plasma states is essential to understand fusion energy. Understanding the molecular, ionic and atomic interaction of reactants is essential to understand the chemistry of energy conversion processes or materials production. Determining the sequence of DNA bases in complete genomes is essential for defining the basic set of RNAs and proteins essential for life, and determining the structures, functions, and interactions of biomolecules is essential for understanding how living systems function, behave, and adapt to changing environments.

Exploring Matter and Energy presents the following major *scientific challenges* for DOE's science portfolio:

Challenges

- ***Components of Matter***—To understand matter at the most fundamental level.
- ***Origins and Fate of the Universe***—To understand the evolution of the universe from fundamental laws.
- ***Complex Systems***—To understand and control complex systems of matter, energy, and life.

DOE manages the world's preeminent infrastructure for basic

Extraordinary Tools for Extraordinary Science
— National assets for multidisciplinary research

research in the physical sciences and an increasingly important infrastructure for chemical and biomedical research. From the large, high energy research facilities, such as colliders, to advanced computational and simulation centers, to the national laboratory system itself, these core resources support multidisciplinary research within DOE and for the nation. Included are the large number of scientific user-facilities that are operated for the express purpose of providing our nation's leading scientists with one-of-a-kind experimental tools for scientific discovery. In providing these extraordinary tools, we must address three key questions:

How can we explore the frontiers of the natural sciences? Challenging questions in the natural sciences often require the application of probes that are capable of peering into the interactions at the sub-atomic, atomic, and molecular scales. Using these experimental probes to unlock the mysteries of matter and energy improves our ability to control these processes and to improve the human condition.

How can we predict the behavior of complex systems? Armed with increasingly powerful mathematical tools and large sets of data from experimental probes and monitoring equipment, scientists can develop super-high-speed computing abilities, create advanced software and visualization systems, and improve their understanding of the complex phenomenon at work.

How can we strengthen the nation's capacity for multidisciplinary science? More and more of the cutting edge of science can be found at the boundaries between technical disciplines. As we search for simpler truths, the process for getting there becomes more complex, requiring the ability to bring together the tools and the different scientists required to solve these problems. Our national laboratories, working in partnership with the private sector and academia, provide unique and powerful settings for conducting multidisciplinary research. In addition, we must be able to exchange information more readily and improve the general scientific literacy of the nation, to lay the foundation for successive generations of world-class scientists.

Extraordinary Tools for Extraordinary Science presents the following major *scientific challenges* for DOE's science portfolio:

Challenges

- ***Instrumentation for the Frontiers of Science***—To provide research facilities that expand the frontiers of the natural sciences.

- ***Scientific Simulation—***To advance computation and simulation as a critical tool in future scientific discovery.

- ***Institutional Capacity—***To strengthen the nation's institutional and human assets for basic science and multidisciplinary research.

The figure in the Executive Summary shows the strategic framework that has been constructed over the past year out of the national discussion of DOE's long-term research directions. The first analytic categories are the four major themes; beneath each of the themes are its three

associated challenges. This organization of themes and challenges is reflected in the twelve chapters of this document; each chapter discusses one scientific challenge. The challenges of "Fueling the Future" are covered in Chapters 1-3. The challenges of "Protecting Our Living Planet" are covered in Chapters 4-6. The challenges of "Exploring Energy and Matter" are covered in Chapters 7-9. The challenges of "Extraordinary Tools for Extraordinary Science" are covered in Chapters 10-12.

Science Investments—A Portfolio Perspective

A distinguishing feature of the Department's basic science, and indeed basic science in general, is that it is primarily knowledge driven rather than application driven. That is to say, its main purpose is to *explore 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*. As such, discoveries usually have broad-reaching, diverse implications, not only for applied R&D and technology, but for other scientific investigations, revealing investments with extremely high leverage and societal benefit. Scientific discoveries resulting from basic research have had an enormous impact on technology development.

Some research activities within the Science Portfolio, although still basic in nature, are more easily understood in terms of potential areas of application that may benefit from corresponding discoveries. For example, some of the work conducted within basic energy sciences falls within this category. There is a usually a strong communication link between scientists engaged in this research and potential downstream beneficiaries, such as the developers of corresponding energy technologies. The research is usually informed, but not limited by, such user feedback and user-defined problems.

In other cases, the research is much more fundamental and exploratory in nature, pressing the limits of abstract thinking and core capabilities in mathematics, computation, and other areas. Even though highly fundamental and exploratory, it too often results in important spinoffs, and certainly improvements in the core capabilities that drive some of the other sciences. An example is research exploring the relationship between energy, matter, time, and space. In general, our portfolio reflects research that is integrated within a continuum of science that supports applied research and technology.

> "Not everything that can be counted counts, and not everything that counts can be counted."
>
> - Albert Einstein

At the outset, it must be noted that the development of **a portfolio in science requires a different approach, or at least a different frame of reference** than that for applied research and technology programs. In the latter case, it is possible to link investments more closely with segments in the industrial sector and/or applied benefits to society that they produce. The issue then becomes one of performing tradeoff analysis of the desired, oftentimes competing objectives. Such an approach is much less valid for science, and most

experts agree that the collective wisdom of the science community and the recommendations of technical advisory committees may do more to inform proper investments in science and subsequent breakthroughs in discovery and knowledge than any quantitative approach ever could. Appropriately then, the quantitative aspects of this analysis are intended to provide some measure of additional insight into the general motivations and framework for our science investments—they are not intended to validate specific science investments.

Further guiding our analysis, eight *major goals* of a balanced portfolio were considered important. They are summarized in the box on the next page.

One of the more important consequences of our portfolio review effort came from our attempt to align our science activities against a new and different long-term strategic framework consisting of themes and challenges. This perspective has enabled us not only to explain, but to think differently across areas of science and program missions. Already new opportunities are beginning to emerge, for example, in the area of complex systems, based on initial multidisciplinary discussions held during our two national workshops and on follow-on activities at the labs and universities. Each of the next twelve chapters, and the appendix, summarize the results of this crosscutting approach to portfolio analysis.

Although many of our portfolio findings are validated by some of the quantitative information contained within this report, it is not our intent to overuse or overinterpret these results. Rather, the broad range of information contained in this report should be reviewed in its entirety and forms the basis for the observations contained below.

DOE provides broad and balanced support for ***science infrastructure***. The DOE national laboratories represent a crowning achievement in an era of scientific discovery. Among the infrastructure that will support science in the future, the national labs reflect our greatest hope and our best opportunities for conducting the broad-based, multidisciplinary research that will be the hallmark of future innovations. Residing at the laboratories and at universities are instruments that enable us to explore scales from the infinitesimally small to the infinitely large, from the sub-atomic to the cosmos. Instrumentation at the Frontiers of Science includes accelerators for high energy and nuclear physics, light sources and neutron beam facilities for natural and life sciences, plasma and fusion energy facilities, single purpose and multidisciplinary facilities, biological and environmental research facilities, and facilities for computing and computational support. Beyond these extraordinary tools of science, DOE invests some highly leveraged resources in science education to ensure that our future scientific workforce is capable of pushing the envelope of science.

Eight Goals for a Balanced Science Portfolio

(1) Support vital science infrastructure, including the national labs and advanced scientific instruments that will ensure the nation's future ability to conduct complex, multidisciplinary science; support a workforce of scientists prepared to meet our future science challenges.

(2) Maintain and build required core competencies, in particular, those vital to our future science programs, such as scientific simulation, anticipating the needs and domains of science.

(3) Provide strong support to DOE's applied research programs, particularly the energy, environmental, and defense missions of the Department, ensuring research is responsive to broad categories of user-defined problems and barriers to technology development.

(4) Support a balanced portfolio across the continuum of science, from exploratory basic research to strategic basic research, the latter informed but not limited by potential applied research problems.

(5) Examine the boundaries of science disciplines, recognizing that some of these offer the greatest potential areas for discovery in the years ahead and that required systems-level investigations/solutions will introduce a higher degree of scientific complexity than ever before.

(6) Collaborate for greater science impact, pursuing international collaborations for large fundamental science investigations and, to the extent possible, industry and university partnerships to increase the leverage of smaller scale, basic research.

(7) Promote diversity of performers and diversity of ideas, working to ensure that an open, competitive process enables the best and the brightest to flourish in a creative science environment, rewarding risk-taking, ingenuity, and excellence in pursuit of scientific discovery.

(8) Expand access to science and to scientific results, ensuring that research facilities and research results are responsive and easily accessible to the scientific community.

DOE's support for ***scientific core competencies*** is best observed in the earlier table that contains the discipline-oriented elements of the budget. Here can be seen the distribution and breadth of support for basic energy sciences, biological and environmental sciences, high energy and nuclear physics, plasma fusion sciences, and computational and technology research, all core competencies that underpin DOE's science mission. In addition, new opportunities have been identified in areas with high leverage, such as scientific simulation. This portfolio demonstrates the interconnected and vital future role of scientific simulation. The Department is preparing a science roadmap for scientific simulation that will clarify the opportunities and options for moving forward in greater detail.

DOE's science portfolio provides strong ***support to the Department's applied research programs*** in energy, environmental management, and national security. For example, research in Fueling the Future maintains a strong eye toward the needs of the applied energy programs. In addition, the strategic framework that includes Fueling the Future was designed to be consistent with the framework adopted in the Energy R&D portfolio, a companion to this report. The Energy R&D Portfolio also includes a detailed chapter outlining the supporting role of science in energy R&D.

Examples of some specific energy technology areas that have benefited from recent strengthened integration between basic science and the applied energy programs include:

- Office of Energy Efficiency's Industries of the Future Program.
- Partnership for a New Generation Vehicle.
- Advanced Computation Initiative, which includes the Office of Energy Efficiency as well as the oil and gas industry.
- Advanced Turbine Systems Program.

Similarly, research that supports challenges in Protecting Our Living Planet strongly supports DOE's environmental management/cleanup mission, and research documented there addresses the need for more timely and cost-effective cleanup solutions. Finally, research in plasma sciences and the general area of scientific simulation are examples of science that also supports our national security mission.

The portfolio ***balances exploratory, fundamental research with strategic basic research***, that is, research with a general class of problems in mind. On the one end of the spectrum, research that supports Components of Matter, as well as Origins and Fate of the Universe, substantiates our continued commitment to the frontiers of knowledge. The heart of this research is exploration—exploration of the cosmos, exploration of the microcosm, but nothing less than exploration of the nature of the physical universe and physical laws that govern energy, matter, time and space. On the other end of the spectrum is work in the Basic Energy Sciences, where, for example, research into new classes of materials or catalysts offers solutions to vexing technology barriers.

This portfolio portrays a major new attempt at strengthening capacity and pursuing opportunities at the ***boundaries of science disciplines***. Support for interdisciplinary science is captured across many of the challenges. For example, pieces of the life sciences are included under Components of Matter, specifically as biomolecular building blocks; and under Origins and Fate of the Universe, life sciences are addressed in the Formation of Life, specifically, simple, primitive organisms and their existence in extremely harsh conditions. The strongest interdisciplinary mix is contained in Complex Systems. Here, research is highly leveraged and builds on ideas spanning many different science disciplines to address collective phenomena and adaptive systems. The challenge of complex systems has received considerable attention, both during our national workshops and in follow up at laboratories and universities.

Many factors make international ***collaboration*** on large science ventures beneficial to the United States. In some cases, the science that underlies the problem is so complex and the impacts so far-reaching that all countries must share in the expense of research. This is the case with Global Change Research. In other situations, the scale and costs of the equipment are so large that even wealthy nations can no longer afford independent activities. In this latter case, the benefits and risks are shared across teaming participants, offering the benefits of new ideas, improved sharing of technical data and science infrastructure, and overall improved communications within the scientific community. The Large Hadron Collider for high energy physics is an example and it demonstrates the sheer physical size and tremendous costs associated with extending research to the next energy level in physics. Also, the U.S. fusion program has similarly exercised leadership in establishing and fostering international collaborations that have involved scientific and technological exchanges, joint planning, and joint work at facilities in the U.S. and abroad. In general, exploratory challenges within Components of Matter and within Origins and Fate of the Universe present many such opportunities for scientific collaborations.

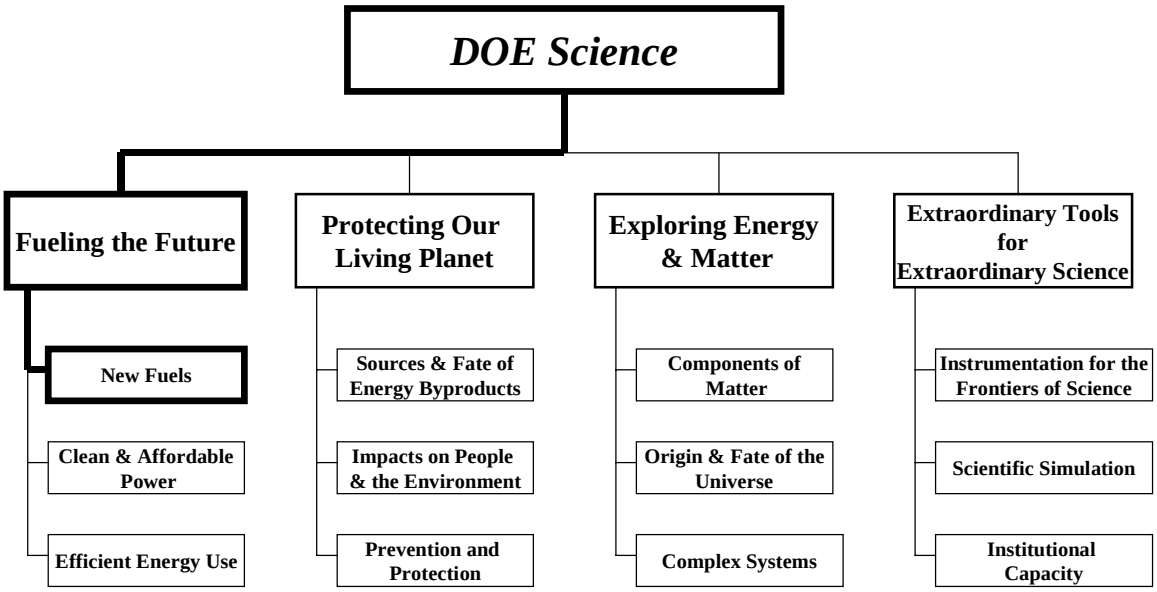
The Department continues to seek ***diversity of ideas and new perspectives on science***. Maintaining a diverse portfolio of research performers is an important component of this overall goal. Researchers at the national laboratories and at universities form the core of DOE-funded scientists, with a larger share going to the national labs. A very sizeable amount went to colleges and universities. Unlike DOE's applied energy programs that have a substantial portfolio investment with industry, the science portfolio invests only a modest amount with industry (see Appendix A), as one might expect given the infrastructure, time-frames of interest, and priorities of industry. Described under the Institutional Capacity challenge, programs and investments designed to broaden the scope of S&T programs/performers has been quite successful. Research sponsored out of one of these programs resulted in findings that were awarded the journal *Science's* 1998 Discovery of the Year—research on the nature and possible fate of the universe.

Finally, and beyond DOE's own research activities, the science portfolio supports ***access*** to its more than 30 major scientific user facilities for many thousands of the nation's scientists, industry researchers, and graduate students. Literally hundreds of colleges and universities and a similar number of companies, as well as many federal labs, are routine users of light and neutron beam facilities, electron microscopy centers, materials analysis centers, and accelerators for high energy and nuclear physics, to name just a few of these advanced tools for science. To assure a

connected science community, the portfolio includes support for ESNet, a high performance network which links computational and experimental facilities to users. ESNet is a critical component of the research infrastructure for the nation. Further improving connections within the science community is the Information Bridge, a system designed to make scientific and technical information more accessible to scientists, technology developers, and the public.

Chapter 2
New Fuels

Scientific Challenge: ***To understand the geological, chemical, biological, and physical processes for clean and affordable domestic fuels.***



Chapter 2
New Fuels

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Most of the goods and services we use in our everyday lives depend for their production on our energy system, which is powered predominantly by fuels. Fuels enable our standard of living, from heating and cooling our homes to growing and preparing food, to transporting us near and far, to manufacturing a plethora of goods. Wood fuels have been used for hundreds of thousands of years. Coal has been mined since the thirteenth century. Oil began to be burned for energy early in the nineteenth century; later in that century, the age of electricity dawned. In the 1950s advanced alloy steels, welding techniques, and large-scale compressors allowed efficient pipeline transport of natural gas, greatly expanding its role in the energy system. All of these fuels are used today to produce energy for human consumption.

Fuel use, however, often has negative consequences, including local and regional pollutants and greenhouse gases; moreover, considerations of energy security prompt the United States to expand the role of domestic fuels. The challenge of the coming decades is to produce the energy needed by the nation while minimizing or eliminating the impact of fuel use on the environment—reducing or removing sulfur and nitrogen compounds, fine particulates, and (perhaps hardest of all) carbon from the fuel or carbon dioxide from the atmosphere.

Developing clean fuels necessitates a wide range of scientific endeavors: geologic investigation of new fossil reserves; biology, genetic engineering, and materials science to develop renewable sources; materials, engineering and chemistry to develop more acceptable energy options; chemistry to remove pollutants from fuels and convert them to other useful products; and mathematics to model and control such processes. In addition, science provides the means to advance our understanding of the effects of energy extraction from fuels and the means to measure, model, and deal with its impacts.

Solar Energy Conversion

Description, Objectives, and Research Performers

The research effort in photochemical energy conversion ranges from the photophysics associated with direct conversion of solar energy to electricity to the photochemical conversion of solar radiation to fuels and specialty chemicals. Related to the photochemistry program but using different techniques is the radiation chemistry research program. A major goal is to obtain molecular level information on chemical reactivity in solution, reactive transient intermediates, the kinetics and mechanisms of chemical reactions and processes at the solid/liquid interface. This research is conducted at national laboratories and universities.

Research Challenges and Opportunities

The program challenges are to understand, at the molecular level, fundamental processes that capture and convert solar energy. Solar photochemical energy conversion offers an attractive alternative to solid state, semiconductor photovoltaic solar cells. Fundamental concepts of light-induced charge separation at the molecular level may be applied to photodriven endothermic reactions for the conversion of light energy to chemical energy. Industrially significant chemicals such as alcohols may be produced from carbon dioxide, or hydrogen from water, or ammonia from atmospheric nitrogen. In addition, photochemistry presents opportunities for altering chemical reaction pathways so that high volume industrial intermediates and specialty

chemicals and fuels can be produced by less polluting processes. In both industrial and specialty chemicals commercial production using solar energy may result in lower financial cost with reduced environmental impact. In regard to global warming, photochemical reduction of CO_2 poses scientific challenges that deserve serious attention. The radiation chemistry research program provides information on intermediates in solution, at liquid/solid interfaces relevant to solar photochemical energy conversion, environmental waste management and remediation, as well as nuclear energy production and catalysis.

Research Activities

The program explores the fundamental concepts associated with understanding photosynthesis focuses on the light-induced charge separation at the molecular level. This understanding is germane to photodriven endothermic reactions for converting light energy to chemical energy. The program encompasses several broad areas, including organic and inorganic photochemistry, electron and energy transfer in homogeneous and heterogeneous media, photocatalysis, and photoelectrochemistry and, hence, examines fundamental issues of chemical reactivity in solution. This research includes biomimicry, or artificial photosynthesis. Naturally occurring photosynthetic reaction centers and antenna systems are studied as models of biomimetic/photocatalytic assemblies that can carry out efficient photoinduced charge separation. Research activities include the spectroscopic investigation of photosynthetic systems at short times following the absorption of light to determine the nature of the excited electronic states involved in the energy conversion process. The radiation chemistry research provides information on transients in solution and intermediates at liquid/solid interfaces for resolving important issues in solar photochemical energy conversion, environmental waste management and remediation, and intermediates relevant to nuclear energy production.

Major research efforts include inorganic photochemistry and electron transfer at Brookhaven National Laboratory; photoelectrochemistry at the National Renewable Energy Laboratory; and photosynthesis at Argonne and the Ames Laboratory. The radiation chemistry program is centered around specialized facilities at the Notre Dame Radiation Laboratory, Argonne National Laboratory, and Brookhaven National Laboratory. The Notre Dame Laboratory serves as the primary user facility for radiation chemistry in the United States.

Accomplishments

- Understanding of the conformational arrangement necessary for initiating charge separation and electron transfer has provided a new basis for development of biomimetic molecules for photosynthesis. A liquid molecule was recently discovered that spontaneously self-organizes into highly ordered ribbon-like crystals, a state known to be important for photoconversion because of the importance of crystallinity in semiconductor films. The electrical conductivity of the film increased sevenfold during the spontaneous transformation.

- Molecular models that duplicate key parameters of the light-energy conversion apparatus of photosynthesis, including charge separation, have been achieved. Supramolecular structures for light harvesting, such as pentameric porphyrin arrays and starburst dendrimers, were obtained and multimetal complexes that feature chromophoric and

catalytic sites were designed and synthesized. Long-lived charge separation has been achieved in a variety of microheterogeneous environments, such as zeolites, layered oxide assemblies, and ordered polymers.

- Theoretical studies on semiconductor nanoclusters successfully predicted their size-dependent optical properties—important for selecting semiconductors to make quantum dots with more efficient optical transitions or as better single electron devices. To make smaller, faster, cheaper components, scientists are investigating nano-scale fabrication techniques. Nanocrystalline semiconductor quantum dots have been exploited for their large surface area and size-dependent absorption characteristics.

- Studies of translationally excited atoms were a staple of the early program in radiation chemistry as it related to nuclear technologies. F. Sherwood Rowland was supported to study such systems, especially hot chlorine atoms. He recognized that photolysis offered an easier path to hot chlorine atom formation, that fluorocarbons were convenient sources and serendipity led him to recognize the impact of chlorine atoms upon the ozone layer, a discovery that resulted in the Nobel Prize in Chemistry in 1995.

- Improvements in the knowledge of behavior of condensed matter physics have been applied to develop photovoltaic solar cells that convert sunlight into electricity with 30% efficiency—far more than the 10-20% efficiencies of earlier devices.

- Paradigm studies of Ruthenium bipyridal complexes have demonstrated the feasibility of photovoltaic, photogalvanic, and chemical photoconversion processes based on this and other inorganic and organic molecular sensitizer systems.

Plant and Microbial Research

Description, Objectives, and Research Performers

The program supports mechanistic research on fundamental biological processes related to capture, transformation, storage, and utilization of energy. Research focuses on the microbiologically driven carbon exchange between the oceans and atmosphere and the exchange between the atmosphere and the terrestrial biosphere and soils. These exchanges have been absorbing much of the anthropogenic carbon released to the atmosphere. Genomic DNA sequences will be determined for microbes capable of transforming sunlight and waste products, including cellulose, into energy, such as methane and hydrogen, at room temperature and room pressure, offering the promise of new energy sources. This research is conducted primarily at universities. A Memorandum of Understanding signed in 1987 established a three-agency plant science partnership (DOE, NSF, and USDA) that jointly solicits and reviews proposals for multi-institutional research coordinating group awards and interdisciplinary research training group awards. In addition, there is an internationally recognized group at the Plant Research Laboratory at Michigan State University, which studies many areas of plant science and uses Arabidopsis as a model plant system. The Complex Carbohydrate Research Center at the University of Georgia provides services and instrumentation for the structural analysis of carbohydrates derived from microbial sources.

Research Challenges and Opportunities

The research focuses on plants and non-medical microorganisms to form a broad scientific foundation for support of the Department of Energy's challenges in energy production, environmental management, and energy conservation. Almost all aspects of energy are immersed in the web of life on earth. Plants, which are a major component of that web of life, can represent an energy demand in terms of producing food and other products, an energy source in terms of biomass or plant-based fuels and chemicals, or a biological filter and digester in terms of exposure to the waste and byproducts of different energy production systems that are released into the air, water and soil. Microbes are also used extensively in various energy-related activities ranging from tertiary oil recovery to the production of alcohol fuels. In nature, microbes have evolved very complex and diverse metabolic and physiological capabilities. The study and understanding of these capacities will permit their full exploitation in an energy context.

Fundamental research in plants and microbes increases our opportunities to understand how carbon moves through the ecosystem and provides concepts on means to impact man's activities, because plants and microbes provide the main route for living system to convert carbon dioxide into higher chemicals. Each of these areas have the potential to be commercially applied, resulting in major economic and societal impacts, such as the formation of a new generation of bio-based industries and a major impact on the nation's production and use of energy-expensive chemicals and fuels.

Research Activities

The focus of research on plants includes photosynthetic mechanisms and bioenergetics in algae, higher plants, and photosynthetic bacteria; control mechanisms that regulate plant growth and development; fundamental aspects of gene structure, function, and expression; plant cell wall structure, function and synthesis; and mechanisms of transport across membranes. Research supported in these areas seeks to define and understand the biological mechanisms that effectively transduce light energy into chemical energy, to identify the biochemical pathways and genetic regulatory mechanisms that can lead the efficient biosynthesis of potential fuels and petroleum-replacing compounds, and to elucidate the capacity of plants to remediate contaminated environments by transporting and detoxifying toxic substances.

The research focus in the microbiological sciences includes the degradation of biopolymers such as lignin and cellulose; anaerobic fermentations; genetic regulation of microbial growth and development; thermophily (e.g., bacterial growth under high temperature); and other phenomena with the potential to impact biological energy production, conversion, and conservation. Organisms and processes that offer unique possibilities for research at the interface of biology and the physical, earth, and engineering sciences are also studied.

Accomplishments

- The composition and structure of pore proteins can now be altered to change the size of the pore, the selectivity of the pore for letting different molecules pass through, and the pore's ability to open and close. Among the potential products of this research are

chemical triggers or molecular switches that can be used to create new sensors to detect harmful chemicals or viruses.

- A chemical in the walls of cells destined to become embryos has been shown to make other nearby cells change their development so that they too are fated to become embryos. This simple cell-to-cell communication shows how a cell can differentiate according to its precise location within the whole plant.

- The DNA sequences of several energy-related microbes have been or are being determined to provide information needed to develop new or improved energy sources that minimize pollution. The microbes being characterized include *Archaeoglobus fulgidus* (which contribute to oil well souring), *Thermotoga maritima* (which may be used in energy generation from biomass), *Methanobacterium thermoautotrophicum* (a methane producer), and *Carboxydothermus hydrogenoformans* (a hydrogen producer).

- Research on fatty acid desaturases and hydroxylases has deciphered the mechanism that controls the introduction of double bonds or hydroxyl groups at specific sites between pairs of carbon atoms in long-chain fatty acids. Identification of the active sites for these enzymes enables the synthesis of new enzymes with specific properties.

- The complete metabolic pathway leading to the bacterial biosynthesis of methane was resolved. The biochemistry of this process was very unusual, involving previously undiscovered cofactors, one-carbon carriers, and enzymes. The novelty of the biochemistry of methanogenesis prompted investigations into the relationship of these bacteria to other known bacteria. These studies concluded that archeabacteria represent a different kingdom of life, a kingdom that was the likely progenitor of both eucaryotes and true bacteria.

- Dr. Paul D. Boyer shared the 1997 Nobel Prize in Chemistry for "elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosphate (ATP)." The energy captured from photosynthesis or released from respiration is converted into the central molecule, ATP, where it is used to maintain cells and synthesize cellular components, as well as for energy-requiring processes such as movement. Dr. Boyer's work, which was sponsored by the Office of Science, examined the detailed chemical reactions involved in the synthesis of ATP and the roles played by specific parts of the ATP synthase molecule.

Geosciences

Description, Objectives, and Research Performers

Geosciences research aims to build the long-term fundamental knowledge base underlying energy technologies of the future. These future energy technologies will involve exploration, enrichment, production, conversion and consumption of energy and mineral resources and generation of technological wastes. Energy and mineral utilization will also require a better understanding of natural processes that will help to minimize anthropogenic perturbations of earth systems. Ultimately, geosciences research impacts control of industrial processes to

improve efficiency and reduce pollution, to increase energy supplies, and to lower cost and increase the effectiveness of environmental remediation at polluted sites. Advances in geophysical imaging are improving the basis for characterizing the distributions of material properties, including layering, mineralogy, lithology, geometry, fracture density, porosity, fluid distribution and type, and composition of the lithosphere. Geophysical methods are achieving higher resolution and greater penetration. This research is conducted at national laboratories, and in industry and universities.

Research Challenges and Opportunities

Research in geosciences focuses on geophysical and geochemical understanding for advancing choices among current and emerging energy and environmental technologies. Fundamental understanding of mineral-fluid interactions will provide a better foundation for oil, gas, and geothermal resource recovery, and for control of energy byproducts and contaminants in groundwater flow. New fundamental physico-chemical property information on rocks, minerals, and geologic fluids will aid in resource recovery and contaminant assessment and monitoring. Extending the applicability of isotopic tracer and geophysical characterization methods will enable evaluation of natural and human-perturbed processes in the geologic environment. The goal is to increase fundamental knowledge of the processes that transport, concentrate, emplace, and modify energy and mineral resources and their byproducts. A major challenge of geosciences research is to develop improved analytical tools for better characterizing earth materials and systems. This is particularly important because earth systems are inherently heterogeneous, multicomponent and multiphase mechano-physico-chemical environments.

Research Activities

Basic research in geosciences includes geophysical and geochemical properties of rocks and minerals (dry, unsaturated, and saturated) determined in the laboratory or in the field (in situ), by direct or indirect techniques. The research is applicable on many spatial and temporal scales of geologic processes. This includes the interrelationships among constituents and their dynamic properties (physical, chemical, and mechanical) and the role of fluid flow as a cause and/or effect. Research is being conducted on fluid transport processes and dynamics (including advanced numerical analyses) and reaction-transport-mechanical properties of fluid-rock systems from the laboratory to the basinal scale. These studies are advancing the understanding of physical transport processes in porous and fractured rocks, leading to predictive capabilities. Research on the physical controls and effects of the dynamic evolution of geologic structures on a local or regional scale are taking advantage of recent developments in geophysical characterization and computational analyses.

Accomplishments

- Novel non-linear inverse modeling has been developed to relate 3-D electromagnetic fields to subsurface fluid distributions and flow. Such non-invasive characterization and monitoring of contaminant fluids in the subsurface remains one of the highest priorities in remediation technology and has implications for resource recovery as well. For example, 3-D images of a salt-water injection test have shown the shape of the salt-water body and locations of maximum permeability through which the salt water has migrated.

- Innovative experimental methods have been developed to evaluate the effects of density-driven and diffusion-driven fluid flow, which is essential for analyzing multiphase flow in geologic systems.

- A new approach to describing the scaling behavior of fault slip-rates during earthquakes has been developed based on analysis of how earth materials respond to stress-state instability across a fault.

- High-resolution mass spectrometry has been developed and is being used to investigate the transport processes, mechanisms, and pathways of heavy metal contaminants, including uranium- and thorium-series isotopes. Scientists can now calculate the residence times of heavy metals in seawater, and better understand the processes by which they are extracted by precipitating sediment.

- Improvements in laboratory, analytical, and numerical modeling have contributed to a better understanding of the origins and evolution of fracture and fault systems under three-dimensional stress-states; these improved models better reflect natural processes and are better able to characterize potential interactions among fractures and faults.

Materials Chemistry

Description, Objectives, and Research Performers

Basic research in materials chemistry includes the synthesis and characterization of complex, multicomponent materials with improved properties through new combinations of atoms and new degrees of complexity. The program emphasizes biomolecular and organic materials research and the self-assembly of structures on a nanoscale to take advantage of the huge number of biomolecular materials and processes. The aim is a fundamental understanding of the behavior of novel materials and structures.

This research is conducted predominantly at national laboratories and universities. Some of the centers of excellence in materials chemistry are (1) the Centers for Advanced Materials in Biomolecular Materials, for Advanced Materials in Polymers and Composites, and for Advanced Materials in Surface Science and Catalysis at Lawrence Berkeley National Laboratory; (2) the Chemical-Materials Collaborating Access Team (ChemMatCARS) for studying surface science at the University of Chicago; (3) a concentration of expertise on Chemical-Vapor Deposition at Sandia National Laboratories (to understand the interplay of chemical reactions and fluid dynamics, develop computer codes to model such processes, and transfer this technology to industry; (4) a concentration of expertise on polymeric superconductors at Argonne National Laboratory; (5) a very strong research group on the synthesis and characterization of inorganic materials at Ames Laboratory; (6) a very strong effort in Biomimetic Materials at Pacific Northwest National Laboratory.

Research Challenges and Opportunities

Materials chemistry provides the primary support for fundamental research in surface science, polymers and organic materials, and for new inorganic materials. The surface science is

important for energy in the understanding which can bear on catalysis as well as surface interactions which lead to degradation and corrosion of surfaces including photovoltaic devices, batteries and fuel cells. New techniques for fabrication of nanocrystals such as the use of inverse micelles may have a big influence on the development of arrays of tunable photoabsorption materials for conversion of sunlight into stored energy. Similarly, the development of synthetic membranes may have uses for separations and for energy storage. Research on solid electrolytes is already paying off in new rechargeable batteries which can be recharged many more times than existing commercial cells. Research on polymers may lead to lightweight structural materials that can be used for automobiles and thereby provide substantial savings in gas mileage, and reduce corrosion. It should be noted that Saturn cars use polymeric door panels which are flexible and bounce back after deformation.

State-of-the-art experimental tools are becoming more available: synchrotron x-ray sources, new and upgraded neutron sources, high magnetic fields, and high pressures. There will be an increase emphasis on nanoscale structures and the way these structures behave chemically. We may see new techniques to develop materials using DNA-type templates. In addition, there will be increased multi-investigator efforts to bring appropriate talent to bear on increasingly more difficult problems.

Research Activities

This program is the primary support in the nation for research in polymers, organic materials, biomaterials, surface science, and new inorganic materials, all of which are important in applications such as fuel cells, batteries, membranes, catalysis, electrochemistry, and photoabsorption. Activities include investigations of low-dimensional structures of self-assembled monolayers, micelles, polymeric conductors, organic superconductors and magnets, complex fluids, colloids, biomolecular materials clusters and nanocrystals, and interfacial phenomena. The research employs a wide variety of experimental techniques to characterize these materials, including x-ray and neutron spectroscopies, scanning-tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and x-ray and neutron reflectometry. The activity also supports the development of new experimental techniques such as double rotation NMR, neutron reflectometry, atomic force microscopy of liquids, and zero field NMR using SQUID detection.

Accomplishments

- A combinatorial chemistry system has been devised for optimization of physical and chemical properties in which the chemical composition of a material can be changed, with each composition located at a point on a grid. The performance of each composition is then tested and the optimized composition can be selected easily and rapidly. This is one of the important new methodologies to reduce the time and costs associated with producing effective, marketable, and competitive new substances.

- Scientists have discovered a broad class of designed organic molecules that self-organize at three hierarchical levels into functional supramolecular materials. The basis for the synthesis of this new class of films is a pencil shaped organic molecule termed a "rodcoil," so named because one-half of the molecule is rigid and the other half is

flexible. This property could make the films useful for everything from anti-icing coatings on airplane wings to anti-bloodclot linings for artificial blood vessels.

- A wide range of experimental and theoretical techniques has been developed and used to investigate the fundamental science of Chemical Vapor Deposition (CVD). The complex chemistry and the complex fluid flow were modeled, experimental detection of reactive gas phase species including molecular beam radical-surface studies was achieved, state-of-the-art CVD reactors were developed, and extensive models easily adapted to specific systems were generated and tested. A new facility at Sandia, established as a result of these fundamental studies, aids CVD reactor manufacturers design better instrumentation.

- Over the past 10 years, new techniques in high resolution nuclear magnetic resonance (NMR) have been developed and applied to scientific problems. Included in a long list of such techniques are: Laser-Polarized Xenon NMR and MRI signal enhancement, making possible sensitive study of structure and dynamics of molecules in solution, on surfaces, and in live tissue; double-rotation NMR, making possible analysis of quadrupole nuclei; zero-field NMR, making possible, when coupled with hyperpolarized Xe, brain and cardiac MRI in the absence of a magnet; and multiple quantum NMR.

- Synthesis and characterization of the first room temperature molecular polymer-based magnet was achieved. This achievement increased the critical temperature of molecular magnets from 19K to ~400K. This result has spawned a new wave of research in this area with a new class of molecular inorganic magnetic materials.

Portfolio Summary

This portfolio area, "New Fuels," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activities that strongly support or moderately support New Fuels, including solar energy conversion, plant and microbial research, geosciences, and materials chemistry. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

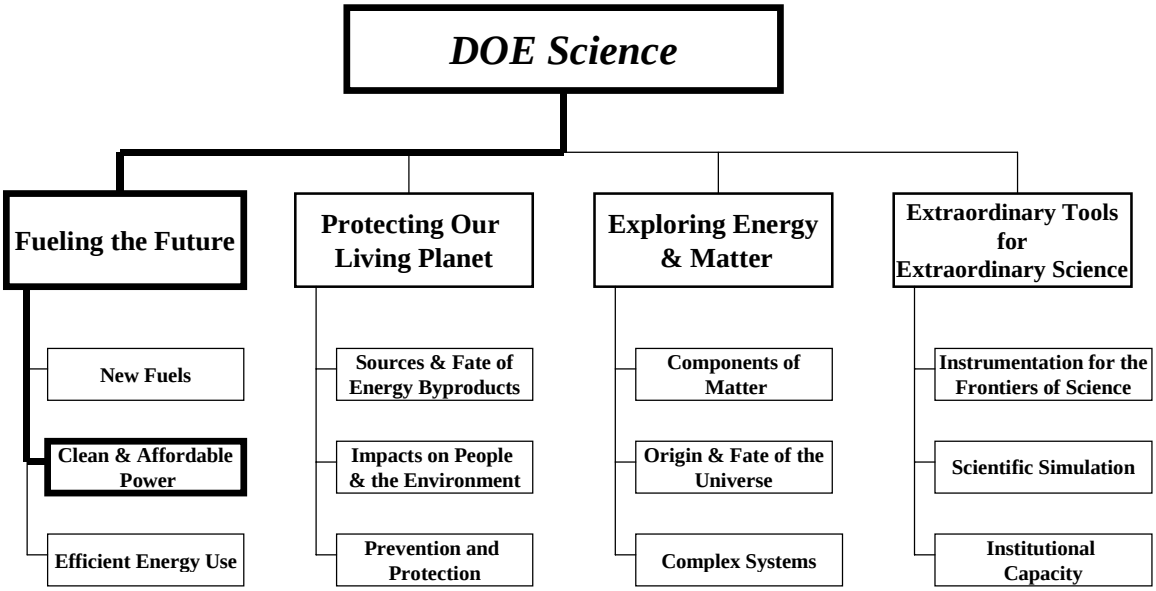
Strongly Supportive Core Research Activities
Applied Mathematics
Chemical Energy and Chemical Engineering
Climate Change Technology Initiative (CCTI)
Energy Biosciences
Geosciences
Materials Chemistry
Microbial Genomics
Photochemistry and Radiation Research

Moderately Supportive Core Research Activities
Advanced Computing Software and Collaboratory Tools
Catalysis and Chemical Transformations
Cleanup Research
Computer Science to Enable Scientific Computing
Environmental and Molecular Sciences Laboratory (EMSL)
Experimental Program to Stimulate Competitive Research (EPSCoR)
General Purpose Plant & Equipment (GPP/GPE)
High Performance Computer Networks
Laboratory Technology Research and Advanced Energy Projects
Multiprogram Energy Lab Facilities Support (MELFS)
Neutron and Light Sources Facilities
Oak Ridge Landlord
Science Education Support
Separations and Analysis
Small Business Innovation Research (SBIR) Program
Small Business Technology Transfer (STTR) Program

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 3
Clean and Affordable Power

Scientific Challenge: ***To understand the physical, material, and chemical processes for advanced power generation, storage, and transmission.***



Chapter 3
Clean and Affordable Power

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New and continued advancements in our scientific knowledge will provide the nation with power that is economically competitive while meeting environmental standards. Clean and affordable power has two focus areas: (1) advanced power systems and (2) enhanced electric utility infrastructure.

The advanced power systems area includes plasma science and all aspects of nuclear fusion. Plasma science is an important element of the scientific infrastructure of the country, and fusion energy is the "grand challenge" of plasma science. Although most of the visible matter in the universe is in the plasma state, plasmas are less common on earth and those relevant to fusion can only be studied in complex laboratory experiments. This is a long-term research and development program with huge potential impact on both advanced power systems and infrastructure in the middle to later part of the next century.

The utility infrastructure focus area is associated predominantly with the basic and fundamental science needed for efficient conversion of chemical and mechanical energy to electric energy, efficient distribution, and final utilization of electrical energy. Research underway that will impact the energy infrastructure of the future includes condensed matter physics underlying superconductivity and transport properties of matter, the engineering of advanced materials for hardness and mechanical stability, materials design for radiation resistance, research on magnetic materials, fundamental understanding of the mechanical behavior of materials, and design of new materials.

Plasma Science and Fusion Research

Description, Objectives, and Research Performers

The process of nuclear fusion - evident in stars, including the Sun - releases enormous amounts of energy. The goal of the program is to advance plasma science, fusion science and fusion technology, and thereby establish the knowledge base of an economically and environmentally attractive fusion energy source. The three objectives of the program are to understand the science of plasmas, identify and explore innovative and cost-effective development paths to fusion energy, and to explore the science and technology of energy producing plasmas as a partner in an international effort. This research is conducted at universities, national laboratories, and industrial firms.

Research Challenges and Opportunities

There are two promising approaches to achieving fusion energy: magnetic and inertial confinement. Theory and simulation of plasma behavior in both magnetic and inertial fusion is complex because of the many orders of magnitude in spatial and temporal scales involved. It is further complicated by the need to understand electromagnetic wave/plasma interactions and plasma material interactions. Magnetic confinement experiments require innovative configurations of magnetic field lines to contain the hot fusion plasmas. Inertial fusion experiments require simultaneous illumination of the full surface of fusion fuel pellets by high-energy beams to create the needed inertial confinement.

The long-term potential for successful commercialization of fusion energy could radically change the overall pattern of electricity generation. Because fusion power plants would not produce air pollutants that contribute to acid rain and that may contribute to global climate change, they could minimize the environmental risks associated with the burning of fossil fuels. Further, because fusion power plants would contain only small quantities of fuel at any time, they could eliminate the potential for runaway reactions that might lead to accidents. The development of low-activation materials or advanced fuel cycles for fusion reactors could make the amounts of high-level radioactive waste that result from fusion-produced energy far smaller than those produced by fission reactors—thus simplifying waste disposal problems.

Although the burning of fusion fuels (deuterium and tritium) does not produce radioactivity, the tritium itself is radioactive, and the neutrons produced by fusion will induce radioactivity in surrounding materials. Although fusion has great potential as a safe and environmentally benign source of energy, there are safety and environmental issues associated with radioactive materials in future fusion devices; these issues will need to be addressed Developing an attractive fusion energy source requires major advances in technologies for plasma and neutron-interactive fusion power core components and in neutron-interactive structural materials with the potential for superior performance in fusion energy systems. The hostile neutron irradiation environment of future fusion power cores will place unprecedented demands on structural materials.

Research Activities

Theoretical and computational research in plasma science provides the predictive capability needed to make progress in plasma and fusion science. Current research areas include plasma turbulence and its effect on the transport of particles and energy in plasmas, macroscopic equilibrium and stability of confined plasmas, edge plasma physics and plasma material interactions, plasma heating and current drive with radio-frequency waves, and understanding the characteristics of innovative confinement configurations. Plasma theory and simulation are also key to understanding other scientific phenomena, such as magnetic reconnection in solar and magnetospheric plasmas or turbulence, chaos, and self-organized behavior in complex systems. Finally, simulation in plasma physics is similar to and promotes progress in fields such as computational fluid dynamics and climate modeling.

The plasma technologies program provides the technology tools needed to create, control, and understand the high-temperature plasma state in fusion experiments. Experiments on the DIII-D and Alcator C-Mod tokamaks are being carried out in combination with continuing theoretical development to dramatically reduce energy losses in these experimental fusion energy systems. An important new facility, the National Spherical Torus (NSTX) began operations in FY 1999. This proof-of-principle level facility will investigate the physics of the promising spherical torus concept. Collaborative experiments with our major international partners will also attempt to scale these results to energy producing plasmas. The experimental program with heavy ion drivers for inertial fusion energy shows promise for significantly advancing inertial fusion science.

Accomplishments

- Significant progress has been made in understanding the behavior of magnetically confined plasmas during the past 10 years. Three-dimensional simulations of microturbulence and the associated energy transport in tokamaks, including the effects of turbulence suppression by zonal flows, agree well with analytic calculations and qualitatively with experimental results. Similar calculations have been carried out for the edge plasma region, and the physics of edge transport barriers is fairly well described.

- Equilibrium and stability calculations combined with current and pressure profile control calculations have identified advanced tokamak operating regimes that are now being explored experimentally. Predictions of instabilities driven by the fusion-produced, alpha particles in a tokamak have been verified in the Tokamak Fusion Test Reactor (TFTR) and the Joint European Torus (JET).

- Credible models of the plasma boundary/divertor regions of a tokamak plasma have been developed, and extrapolations to burning plasma devices are becoming increasingly reliable. These accomplishments in understanding the behavior of magnetically confined plasmas put scientists one step closer to developing an economically and environmentally attractive fusion energy source.

- Extensive new computational tools to help with the design of alternative fusion confinement configurations, particularly stellarators, have been developed and applied to the design of a new generation of small-scale experiments.

- The heavy ion driver single beam, multiple beam and focusing experiments are demonstrating the scientific basis for induction accelerators in the fusion science program.

Condensed Matter Physics

Description, Objectives, and Research Performers

Research in condensed matter physics is aimed at gaining a fundamental understanding of the behavior of materials. Experimental measurements seek to determine electronic structure, transport properties, phase transitions, mechanism for high temperature superconductivity, complexity in electronic interactions, and self-organization of electronic states. This includes fundamental measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. This activity also supports basic research in theory and simulations of condensed matter, the use of ion beams to study and modify the properties of materials, and engineering applications. The theory activity complements much of the experimental work by guiding, stimulating, and explaining experiments. It includes the support of selected centers with specific materials-related missions. These centers excel in bringing together individual scientists from widely different backgrounds to work on common research areas or make use of common research tools. Included among these are the Center for X-ray Optics and the Centers for Advanced Materials at Lawrence Berkeley National Laboratory and the Surface Modification and Characterization Facility at

Oak Ridge National Laboratory. This research is conducted at national laboratories and universities.

Research Challenges and Opportunities

The major unresolved research question in condensed matter physics is the physical mechanism that makes high temperature superconductivity possible. Another issue relates to giant or colossal magnetoresistance. A major challenge is the theoretical understanding of high temperature superconductivity, and of the electronic structure and properties of complex, multicomponent materials.

Future efforts will include continued support for investigations of materials with increasingly complex behavior, composition and structures with strongly competing interactions among the electronic charge and spin, and the crystalline lattice. A major new activity will be the synthesis and fabrication of unusual materials systems with pulsed laser ablation epitaxy, self-organized structures, and engineered materials and structures to provide insight into unusual behavior.

Research Activities

The materials examined include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The measurements include optical and laser spectroscopy, photoemission spectroscopy, electrical and thermal transport, thermodynamic and phase transition measurements, nuclear magnetic resonance, and scanning-tunneling and atomic-force microscopies. The development of new techniques and instruments, including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy, are major components of this activity. Measurements will be made under extreme conditions of temperature, pressure and magnetic field.

The program supports items such as lasers, scanning-tunneling microscopes, electron detectors for photoemission experiments, sample chambers, superconducting magnets and computers. Activities include the design and construction of new, unique research instruments, such as the 100 Tesla Pulsed Field Magnet and the actinide photoelectron spectrometer at Los Alamos National Laboratory.

The emphasis in engineering physics is on the use of fundamental science to advance technology. Engineering physics includes activities such as the application of sound waves for refrigeration; the fabrication of small, machined structures using x-rays; and the development of new, electron microscopy techniques such as the Z-contrast electron microscope at Oak Ridge National Laboratory.

Accomplishments

- First proof of a thermodynamic first-order transition from a solid-like vortex lattice to a liquid in a high-temperature superconductor is leading to development of a new state of matter called vortex matter. The nature of this transition is significant for fundamental theories of phase transitions and for practical applications of

superconductivity. For example, movement of the vortices in response to an electric current dissipates the energy of the current—the resistivity is not zero—and the material is not superconducting.

- Improvements in our knowledge of behavior of condensed matter physics have been applied to develop photovoltaic solar cells that convert sunlight into electricity with 30% efficiency—far greater than the 10-20% efficiencies of earlier devices.

- The discovery of a new electrolyte system, lithium phosphorus oxynitride, which is stable in contact with lithium metal, has enabled the development of thin-film batteries approximately 10 microns thick which have unsurpassed energy densities and can operate safely at temperatures as high as 150 degrees C.

- It was discovered that when nickel is cold rolled into a thin film of superconducting material, the crystalline grains tend to line up and produce oriented films, which allows relatively long lengths of HiTc conducting tape to carry substantial amounts of electric current.

- A novel surface diffusion process first predicted by theory was verified by electron microscopy and has become an important consideration in all modern treatments of surface diffusion. Surface diffusion plays a key role in phenomena such as crystal growth, thin film stability, and chemical reactions.

- Certain three dimensional periodic structures have been shown to possess a photonic bandgap, i.e., a frequency region where the propagation of electromagnetic waves is forbidden for all wave lengths. These structures show promise as antennas, resonant filters, and detectors. This photonic effect results from the contrast in the dielectric properties between the material and air, and is an example of how geometry can play a powerful role in the behavior of materials.

- Quantum mechanical calculations have led to the prediction of the existence and properties of yet unknown materials, e.g., C3N4, which rival diamond in hardness. If efforts to synthesize these materials are successful, they would provide options for new coatings, abrasives, and cutting tools.

Metal and Ceramic Sciences

Description, Objectives, and Research Performers

This activity supports fundamental experimental research that specifically targets the needs of the DOE technology programs and, therefore, has significant impacts on energy generation, transmission, conversion, and conservation technologies. The work conducted in this program is long-term fundamental research in materials, with a focus on the influence of synthesis and processing on the materials' structure and properties. Mechanical behavior and radiation damage are also studied to understand the fundamental principles of the defect-property relationship on an atomic level, so that predictive models can be developed that will permit the design of materials that have desired mechanical behavior and resistance to irradiation damage.

Linkage of materials' structure at the atomic level to behavior at the continuum level will become a reality, thus bringing new rigor to the science of mechanical behavior. This research is conducted predominantly at national laboratories and universities.

Research Challenges and Opportunities

Many critical unresolved issues concern the mechanical behavior of materials that have been with us for a long time, but have not been subjected to contemporary multidisciplinary investigation. As in other areas of materials science, recent developments in diagnostics and computation are enabling researchers in mechanical behavior to probe regimes that had not previously been accessible to them. Real time *in-situ* diagnostics now available with programmed mechanical behavior response measurements permit the observation of the evolution of the structure of materials during deformation. The computational capabilities of massively parallel processors allow the simulation of multiple simultaneous processes at different lengths of scale, thus providing a new opportunity for fundamental discovery of deformation mechanisms. Intense and tunable X-ray beams and small angle scattering capabilities also offer myriad opportunities for the in-situ characterization of deformation mechanisms. The challenge is to synthesize these new insights into mechanistically rigorous, validated, predictive models.

The impact is clear—mechanical behavior and radiation effects phenomena underpin the structural reliability and safety of energy generation, conversion, transmission, and conservation systems. Mechanical and irradiation-induced failures may lead to, for example, the escape of undesirable fluids or gases into the environment. In an age when economy necessitates life extension, the ability to predict performance reliably (from a fundamental basis) is becoming key.

Research Activities

Activities include the synthesis and processing of materials with new or improved behavior and/or with reduced waste byproducts; hard and wear-resistant surfaces to reduce friction and wear; high-rate, superplastic forming of lightweight, metallic alloys for fuel-efficient vehicles; and high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools and fuel-efficient and low-pollutant engines. Quantitative, non-destructive analysis provides early warning of impending failure, prediction of remaining reliable service life, and on-line, in-situ flaw detection during fabrication or production. Response of magnetic materials to applied static and cyclical stress is investigated. Research into plasma, laser, and charged particle beam surface modification should yield increased corrosion or wear resistance. Another research area involves processing of high-temperature, high-strength yet fabricable intermetallic alloys; and welding and joining of alloys, ceramics, and dissimilar materials.

Mechanical behavior activities include investigations of deformation and fracture mechanisms, mechanical load-bearing ability, failure and cyclic fatigue resistance, stress-corrosion, high strain-rate behavior, fracture toughness and impact resistance, high-temperature strength, creep-fracture and dimensional stability, and deformation behavior and formability. Radiation effects activities include investigations of mechanisms of neutron irradiation damage and ion implantation into solid surfaces, modeling, predicting and controlling neutron radiation

damage, irradiation-assisted stress corrosion cracking, and surface modification by ion implantation. Significant research that brings together basic and applied researchers takes place under the distributed Center of Excellence for the Synthesis and Processing of Advanced Materials.

Accomplishments

- A new model for electrical resistance spot welding utilizes a unique incrementally coupled finite element modeling approach that takes appropriate account of the deformation and consequential change in the shape of welding electrode contact surfaces.

- Stronger and cheaper magnets have been produced by adding titanium and carbon to a molten neodymium-iron-boron alloy, which permits a spray atomization process to produce nanocrystalline composite powder with a crystallite size that matches that of the magnetic domains in this alloy, which in turn causes this material to produce stronger and cheaper magnets.

- A uniform three-dimensional coating process known as plasma immersion ion processing has been developed. It results in the production of hard coatings, such as diamond-like carbon, that exhibit low sliding-friction and superior wear resistance. Coatings produced by this process may easily be scaled to large areas (many square meters), are uniform over irregular surfaces, produce adherent coatings on a wide variety of substrates, and are economical.

- Research demonstrated that commercially important self-reinforced silicon nitride ceramics must be tailored at the microscopic and atomic levels. This resulted in the formation of low aluminum and oxygen surface layers which in turn yielded an exceptionally high fracture resistance in this ceramic.

- Combining surface-sensitive synchrotron X-ray diffraction with in-situ real-time electrochemical experiments revealed the surprising discovery that the passive oxide that forms on pure iron or on stainless steel has a very fine-grained “nanocrystalline” structure. This startling conclusion overturns the long accepted belief that stainless steel is corrosion resistant because the passive film was thought to be non-crystalline.

Energy Production, Storage and Transmission

Description, Objectives, and Research Performers

This activity addresses energy aspects of chemically related engineering sciences, including thermodynamics, turbulence related to combustion, and physical and chemical rate processes. Particular attention is given to experimental and theoretical aspects of phase equilibria, especially of mixtures, including supercritical phenomena, and to the physics of gas phase turbulence. Also included are fundamental studies of thermophysical and thermochemical properties. Emphasis is given to improving and/or developing the scientific base for engineering generalizations and their unifying theories. Also included is fundamental research in areas critical to understanding the underlying limitations in the performance of

electrochemical energy storage and conversion systems. Areas of research include the characterization of anode, cathode, and electrolyte systems and their interactions. The program covers a broad spectrum of research, including fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces.

The aim is providing knowledge that will lead to improvements in battery size, weight, life, and recharge cycles.

Research Challenges and Opportunities

A major challenge is to understand the fundamental chemical engineering sciences that underpin nearly all energy intensive chemical processes. In this regard, particular emphasis is placed on electrochemical storage and conversion, and turbulence both in combustion and in fluid flow. New opportunities have been identified associated with the need to couple the current emphasis of the program in molecular simulations with molecular level theory. This new knowledge will reduce the uncertainty in calculations and provide a better molecular-level basis for engineering generalizations and theoretical tools. Development of a molecular-level understanding of the physical and chemical processes is important to the environmentally benign utilization and conversion of our fossil energy resources.

Research Activities

Fundamental research in energy aspects of chemically related engineering topics using advances in molecular and statistical mechanics, quantum chemistry, and molecular simulation emphasizes improving and/or developing the scientific base for engineering generalizations and their unifying theories. Fundamental research critical to understanding the underlying limitations in the performance of electrochemical energy storage and conversion systems focuses on the study of the electrochemical interactions of electrochemical couples and electrolytes at heterogeneous and buried interfaces. Although the focus of the Office of Science research is on non-automotive electrochemical energy storage and conversion systems, the fundamental knowledge gained may have broad application.

Accomplishments

- Fundamental research in the deposition of reactive metals and their mobility and stability in non-aqueous electrolytes identified those organic electrolytes that led to the development of the current generation of high energy and power lithium and lithium ion batteries. Because of their performance advantages, they are now widely used in consumer and defense applications and are under further development for use in electric vehicles.

- Research has resulted in a new solid polymer electrolyte system that exhibits high room temperature conductivity. This advance resulted from the ability to minimize the strength of the interaction between the lithium complex and the polymer network by controlling the void volume of the network and the hydrophobicity of the interface.

- Fundamental research in ion transport in glassy solids has led to the successful development of thin film lithium battery technology, producing batteries half the thickness of household plastic wrap.
- Basic research in non-aqueous liquid electrolyte systems has led to an approach for prevention of the oxidation of alkali metal electrodes by the electrolyte. This has led to the development of a non-flammable organic liquid electrolyte for lithium and lithium ion battery systems; the modified electrolyte has improved the safety of rechargeable batteries.

Portfolio Summary

This portfolio area, "Clean and Affordable Power," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activities that strongly support or moderately support clean and affordable power, including plasma science and fusion research; condensed matter physics; metal and ceramic sciences; and energy production, storage, and transmission. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

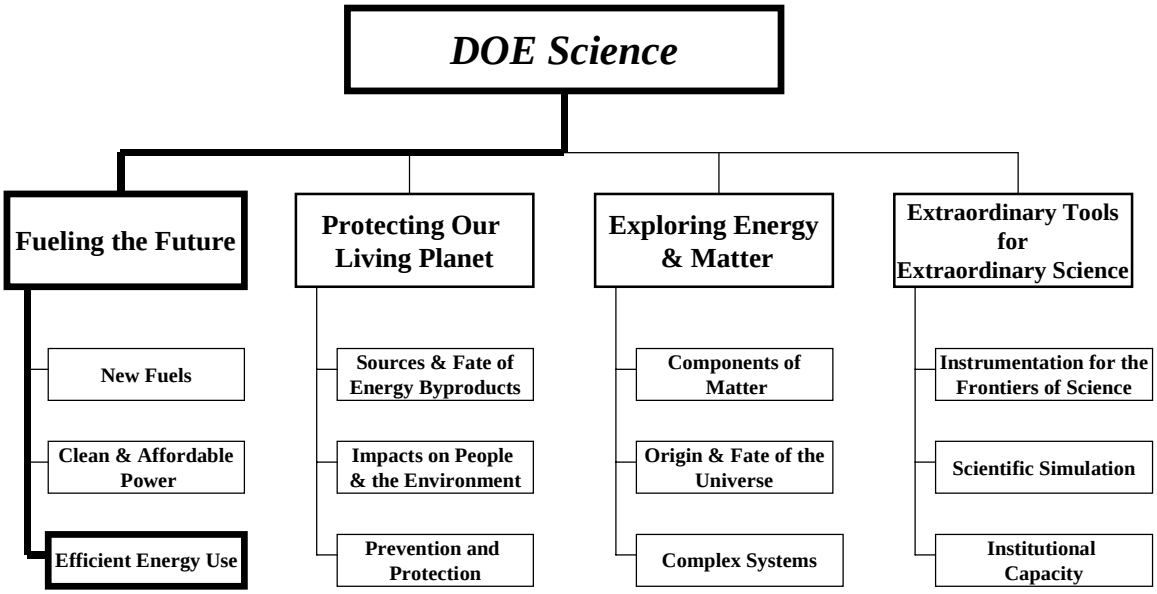
Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations
Advanced Fusion Design
Advanced Fusion Materials Research
Alcator C-Mod Facility Operations
Chemical Energy and Chemical Engineering
Climate Change Technology Initiative (CCTI)
DIII-D Facilities Operations
Engineering Behavior
Experimental Condensed Matter Physics
Experimental Fusion Physics Support
Experimental Plasma Research (Alternatives)
Fusion Physics Research on Alcator C-Mod
Fusion Physics Research on DIII-D
Fusion Physics Research on NSTX
Fusion Technologies
Inertial Fusion Energy Research
Mechanical Behavior and Radiation Effects
NSTX Facility Operations
Plasma Technologies
Plasma Theory and Computation

Moderately Supportive Core Research Activities
Advanced Computing Software and Collaboratory Tools
Atomic, Molecular, and Optical Science"
Chemical Physics Research
Cleanup Research
Computer Science to Enable Scientific Computing
Experimental Program to Stimulate Competitive Research (EPSCoR)
General Plasma Science
General Purpose Plant & Equipment (GPP/GPE)
High Performance Computer Networks
Laboratory Technology Research and Advanced Energy Projects
Mechanical Systems, Systems Science, and Engineering Analysis
Multiprogram Energy Lab Facilities Support (MELFS)
Neutron and Light Sources Facilities
Oak Ridge Landlord
Physical Behavior of Materials
Science Education Support
Small Business Innovation Research (SBIR) Program
Small Business Technology Transfer (STTR) Program
Structure of Materials
Theory & Simulations of Matter, Engineering Physics

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 4
Efficient Energy Use

Scientific Challenge: ***To understand the engineering, materials, and chemical processes to develop new energy efficient technologies.***



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Increasing the efficiency in the way we use energy has only positive effects. Energy efficiency lowers costs, making financial resources available for more productive use. It decreases our dependence on energy supplies from unstable regions of the world. It decreases the adverse affects on the environment from extracting, refining, transporting, and combusting fuels. Also, since the vast majority of the fuel consumed today is carbon based, efficiency is the quickest and most effective way to reduce the principal greenhouse gas—carbon dioxide—and local air pollutants such as particulates, SO_x, and NO_x.

There are many ways to increase efficiency. Some are very simple, such as increasing insulation and caulking leaks. More sophisticated and more difficult ways require substantial basic research and development. Increasing the temperature of heat engines will increase efficiency, but all of the degradation reactions, such as corrosion, increase exponentially with temperature. Understanding combustion reactions will lead to significant improvements in boilers and internal combustion engines. Lowering weight in automobiles and trucks will increase fuel economy, but low weight materials may not be very strong. A large amount of energy is used first to refine, melt, and cast parts only to grind way substantial amounts to create the final shape. Substantial efficiency could be gained with better materials and processes that could cast directly to final shapes. Vast amounts of energy are wasted because of inefficient separation and unspecific catalytic processes. New superconductors can eliminate electrical transmission losses and improve the efficiency of generators. A diverse portfolio of high-quality basic research projects enables the interdisciplinary work needed to solve the problems of efficient energy use. Office of Science research programs help guarantee that energy technology development is being conducted with benefit from advanced scientific knowledge and that basic research projects are focused in areas directly relevant to energy systems.

Combustion-Related Sciences

Description, Objectives, and Research Performers

The research program investigates, at the molecular level, chemical reactions in the gas phase, at surfaces, and at interfaces and the relationship between molecular scale phenomena and bulk phenomena. Research activities involve closely coupled experimental and theoretical efforts. Experimental projects include studies of molecular dynamics, chemical kinetics, spectroscopy, clusters, and surface science. The goal related to energy efficiency is to increase the efficiency of the combustion process.

Combustion-related chemical physics research is conducted at several national laboratories (including a single-purpose laboratory devoted to combustion, the Combustion Research Facility (CRF) at Sandia National Laboratory) and at a broad spectrum of universities. Cluster research is carried out at both national laboratories and universities, while work related to the solid-liquid interface and the relationship to environmental remediation issues is performed predominantly at national laboratories.

Research Challenges and Opportunities

Nearly 90% of the nation's energy needs are produced by combustion. Typical combustion reactions involve dozens, sometimes hundreds, of chemical reactions whose rates at combustion

temperatures must be known. It is not practical to measure all of the rates of reactions that might be included in a computer model for a particular combustion system with a particular fuel and oxidant. One of the challenges of the chemical physics program is to provide data and techniques for producing or predicting the values of chemical reaction rates to be included in combustion models for predicting the efficiency and emission characteristics of combustion devices and for optimization and control of combustion devices.

Catalysis not only makes the production of chemical feed stocks and fuels economically feasible, it does so by reducing the demand for energy. Catalysts also find extensive use in pollution reduction. In contrast to those technical areas that are highly codified with a great deal of predictive capability, surface mediated catalysis is in a more Edisonian stage of development. The surface science and clusters projects in the chemical physics program are aimed at providing predictive capability for surface mediated catalysis through provision of explanatory theories relating surface structure to surface mediated chemistry.

Research Activities

A primary goal of the chemical physics program is to provide combustion-related data and techniques for producing or predicting the values of chemical reaction rates to be included in combustion models. Research activities focus on improving theory and obtaining confirmatory experimental measurements of the dynamics and spectroscopy of vibrationally and electronically excited species relevant to combustion systems to enable predictions of reaction rates under a wide variety of conditions, including high temperatures and pressures, energy transfer phenomena, and spectra for diagnostic probes. Models can then predict the efficiency and emission characteristics of combustion devices, and researchers can optimize and control combustion processes.

The surface science and clusters research is aimed at providing predictive capability for surface-mediated catalysis through provision of explanatory theories relating surface structure to surface-mediated chemistry. Clusters provide a means of relating surface structure to chemical activity because structure is a function of cluster size. The use of a chemical physics approach to investigate fundamental issues at the solid-liquid interface related to environmental remediation issues is also part of this program. The program comprises combustion-related chemical physics research, cluster research, and work related to the solid-liquid interface and this relationship to environmental remediation issues. Experimental techniques are used to determine the structures, while theory is employed to predict the dynamics of surface reactions.

Accomplishments

- Within the last three years a novel and elegantly simple experiment has been designed and refined that allows the interaction of chemistry and turbulence to be examined in quantitative and verifiable detail for the first time. Comparisons of these experiments with computational simulations have shown that the widely accepted chemical reaction mechanism for methane combustion is in error. Because of the simplicity of this experiment, it promises to be widely copied and in the coming years we can expect to see an acceleration in our ability to understand and control combustion processes.

- Scientists have demonstrated a new variant of laser frequency modulation spectroscopy that is specifically tailored to the detection of transient combustion species. Although frequency modulation has long been used to compensate for source fluctuations in spectroscopy, the new technique is simple to apply and likely to gain wide usage. It has already been applied to the study of the chemistry of NH_2 radicals. With this new technique, more rapid progress in the characterization of combustion reaction mechanisms can be expected.

- In studying water and organic solvents adsorbed on surfaces, scientists have observed a phenomenon they have dubbed "molecular volcanoes." The research is conducted to understand, at a molecular level, processes that control movement of organic solvents in soils and aquifers. The knowledge gained will contribute to the development of control and storage strategies for organic wastes.

Advanced Materials

Description, Objectives, and Research Performers

Research in advanced materials is concerned with the microstructural aspects of geometrical packing configurations of atoms in solids, defects and imperfections in those packing configurations, and the microscale morphology and composition of crystalline solids. The objective is to develop quantitative models and theories depicting the structure of materials because that structure, in turn, relates to and controls their behavior and performance. Advanced materials research also includes engineering behavior with a focus on the influence of synthesis and processing on materials structure and properties. Physical behavior of materials is concerned with understanding the mechanisms for various forms of physical behavior, particularly under conditions that interact with and change the bulk and/or surface structure of the material. The objective is to predict physical behavior by developing mechanistically rigorous computational models of materials response under imposed electrical fields and thermal and environmental stimuli, drawing upon fundamental structural models and theories as needed. The basic research program specifically targets the needs of the DOE technology programs and, therefore, has significant impacts on energy generation, transmission, conversion, and conservation technologies. This research is conducted at national laboratories and universities. Significant research that brings together basic and applied researchers takes place under the distributed Center of Excellence for the Synthesis and Processing of Advanced Materials.

Research Challenges and Opportunities

The challenge lies in improving the understanding of the structure of materials and the relationship of structure to behavior and performance to such a degree and extent that this understanding will form the basis for predictive models. These predictive models would then be used to improve the behavior and performance of existing materials or to design new materials with superior behavior and performance. Other challenges are to understand the mechanisms and dependencies of physical behavior and their responses to perturbing stimuli or fields such that valid predictive models or simulations can be developed. These models will help to accurately predict the physical behavior of materials under untested perturbing stimuli or for new and yet unknown materials. Sound predictive models or simulations are likely to guide research

efforts toward more significant discoveries, and in a more cost-effective manner than is currently possible.

Research Activities

Activities include the synthesis and processing of materials with new or improved behavior and/or with reduced waste by-products; hard and wear resistant surfaces to reduce friction and wear; high-rate, superplastic forming of lightweight, metallic alloys for fuel-efficient vehicles; and high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools and fuel-efficient and low-pollutant engines. Quantitative, non-destructive analysis provides early warning of impending failure, prediction of remaining reliable service life, and on-line in-situ flaw detection during fabrication or production. Response of magnetic materials to applied static and cyclical stress in investigated. Research into plasma, laser, and charged particle beam surface modification may yield increased corrosion or wear resistance. Another advanced materials research area pertains to the processing of high-temperature, high-strength, yet fabricable intermetallic alloys; and to the welding and joining of alloys, ceramics, and dissimilar materials.

Predictive theory and modeling covers density functional, coherent potential, pseudopotential, linear combination of atomic orbitals, tight-binding, Monte-Carlo, cluster variation and other methods. Bulk metallic glasses, buckeyballs, dimensionally restricted structures and other forms of new materials are being investigated, and crystal growth, solidification and solid state phase transformation mechanisms. Crystalline defects are being characterized by existing and improved techniques of electron beam microcharacterization, atom-probe field ion microscopy, atomic force microscopy and positron annihilation spectroscopy; emphasis is on improving the precision, detectability, spatial resolution and range of validity of these techniques. Analysis and modeling are being employed to study grain boundaries, interfaces, and free surfaces. Surface phenomena are also being examined. Scientists are studying aqueous, galvanic, and high-temperature gaseous corrosion. Studies of photovoltaics and semiconductors and their junctions and interfaces are contributing to solar energy conversion, sensors, radiation detectors and other solid state devices. Scientists are studying the relationships between and among crystal defects, grain boundaries, and processing parameters to critical current density, fabricability, and other parameters of superconducting behavior for high-temperature superconductors. Phase equilibria and kinetics of reactions in materials are being studied in hostile or extreme environments such as the very high temperatures and reactive environments found in energy conversion processes and in systems that are far from thermodynamic equilibrium, e.g., steels, precipitation hardened or quenched alloys, glasses, spinodal systems, and composites; nanophase systems and finely divided powders; and diffusion and transport of ions in solid electrolytes for improved performance in batteries and fuel cells.

Accomplishments

- Very high quality films and crystals of controlled defect containing complex oxides have been grown that will improve power density and voltage in lithium-containing batteries.

- A breakthrough in understanding the processing of ceramic aerogel films has led to a new non-toxic, low temperature process to produce such films in an environmentally benign manner.

- A new understanding of how hard nitride films are formed has enabled a process to grow diamond-like cubic boron-nitride films, the second hardest known material. Unlike diamond, boron-nitride does not react with iron or steel, making it an ideal material for long-life high-speed cutting tools.

- A tenfold increase in the electrical conductivity of gallium arsenide semiconductors was achieved by creating vacant arsenic sites on the crystal lattice of gallium arsenide which act as “traps” for carbon ions. Carbon-doped gallium arsenide is a semiconductor that is attractive for application in electronic devices, such as diode lasers for reading compact discs or ultra-high speed transistors.

- A threefold increase in the fracture toughness of the structural ceramic silicon carbide was achieved by developing a sintering process that permitted a structure of interlocking plate-like grains to grow during the sintering process. This interlocking structure exhibits exceptionally high resistance to the passage of a crack, thereby increasing the fracture toughness.

- A record solar photovoltaic efficiency of 30% was achieved by acquiring a fundamental understanding of the conversion of solar energy to electrical energy by thin-film semiconductor structures, a newly developed film growth technique, and a tandem, two-stage design based on two complementary solar cells grown as one combined cell.

- Light bulbs, fluorescent tubes, and neon lights may soon become things of the past, replaced by more efficient and brighter lighting sources utilizing light emitting diodes (LEDs) based on gallium nitride semiconductors. A high-pressure spectroscopic method showed that the unexpected high excess of electrons in the manufacturing process for these semiconductors resulted from an oxidizing impurity in gallium nitride, providing a scientific basis for improving the manufacturing process for very efficient LEDs.

Engineering Sciences

Description, Objectives, and Research Performers

Research in engineering sciences is necessary to help resolve the numerous engineering issues that arise from energy production and use. Research includes work in three technical areas: (1) mechanical systems, including fluid mechanics, heat transfer, and solid mechanics; (2) systems sciences, including process control, instrumentation, and intelligent machines and systems; and (3) engineering analysis, including nonlinear dynamics, data bases for thermophysical properties, models of combustion processes for engineering applications and foundation of bioprocessing of fuels, and energy-related waste and materials. This research is conducted principally at national laboratories and universities.

Research Challenges and Opportunities

The research challenges are to extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and to broaden the technical and conceptual base for solving future engineering problems in energy technologies.

Research Activities

In mechanical systems, research activities include seeking a better understanding of diffusion at a flowing gas-liquid interface, experimental testing of the newly developed method for fracture mechanics, and a better understanding of the engineering of nanoscale systems. In systems sciences, ongoing research seeks to relate the operations of the system to the design process in complicated nonlinear chemical processing systems. In engineering analysis, porous silicon is being studied to enable its use in computer systems along with quantum dots as active elements. Scientists need to better understand the shot noise in nano-electronics and electron wave guides in nano-systems with a few electrons.

Accomplishments

- Methods to control the highly unstable chemical processes in very high-pressure reactors for low-density polyethylene production were developed; these methods are now used to prevent shutdowns of industrial reactors.

- Phenomenological understanding that relates large-scale behavior to small-scale interactions between phases led to improved methods for universal predictions of gas-liquid flow in pipelines. This will improve pipeline design and reduce failures.

- A very fast algorithm for many variables was developed for optimizing/minimizing a variety of industrially used systems; use of the algorithm for oil exploration earned an R&D 100 Award.

- A technique was developed to do a visualization of 3-D chaotic mixing. Results from the experiment compare favorably with computer simulations. Such diagnostics will be very useful for better understanding industrial mixing and will provide ways to lower costs in a diverse range of energy-intensive manufacturing processes.

- A new way to capture and focus light was developed, which founded a new field of optics. This led to better solar energy systems, such as a solar furnace operating at almost the temperature of the surface of the sun. Other practical benefits include safer and brighter tail lights on automobiles, a new light condenser for movie projectors twice as bright as previous ones, diodes that replace incandescent bulbs, protective counter measures for military aircraft and tanks, brighter screens for laptop computers and improved flat-panel TV screens.

Catalysis and Chemical Transformations

Description, Objectives, and Research Performers

Basic research in this area is related to the fundamental understanding of chemical transformations and conversions central to new or existing concepts of energy production and storage. The emphasis is on understanding the fundamental chemical principles. Catalysis is a chemical process found widely in nature and used extensively in industry because it removes energy barriers to chemical reactions. Catalysts used for refining petroleum or manufacturing chemicals are important because they reduce process energy, speed up production, and make possible the manufacture of new materials. Models for catalytic action are limited in scope and applicability. The catalysis program seeks to gain understanding of catalysis at the molecular level to allow the development of general theories and models of catalytic action. The program includes both heterogeneous (multiple phases such as liquid/solid) and homogeneous (single-phase) catalysis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes. The program constitutes the largest single component of the nation's basic research portfolio focused on chemical catalysis. This research is conducted at national laboratories and universities.

Research Challenges and Opportunities

New opportunities are in aqueous catalytic chemistry, understanding the interface between water and catalytic oxides, and in catalytic activation and conversion of chlorofluorocarbons. Another area is the development of catalysts and catalytic processes for the transformation of carbon dioxide, i.e., the development of chemistry for new or improved CO_2 mitigation concepts. The disciplines of organic, organometallic, inorganic, physical, and thermochemistry are central to these programs. Despite their importance, catalytic processes are not sufficiently well understood to allow rational design of new catalysts. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added products. The creation of new organometallic precursors has the potential provide materials that are synthesized by less-energy-intensive processes and function as energy-saving media themselves.

Research Activities

Of particular interest are research activities with the objectives of understanding the chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources, particularly coal, including characterization and transformation; the conversion of biomass and related cellulosic wastes; and the chemistry of precursors to advanced materials. Researchers use state-of-the-art methods to elucidate phenomena occurring at aqueous oxide interfaces with emphasis on the nature of species as they undergo the transition from solvation to surface adsorption. They determine new ways to create materials precursors, molecules that will allow the design of materials with specific physical and chemical properties. Researchers develop

methods for detecting single molecular events. They create new multifunctional catalytic systems, bringing together the two basic disciplines of homogeneous catalysis and heterogeneous catalysis. Scientists study materials that are partially ordered, and understand the consequences of short-range order on molecular phenomena related to these materials. They develop tools to probe reaction-induced surface structure dynamics and develop combinatorial approaches to increase the efficiency of gaining fundamental understanding of catalytic processes.

Accomplishments

- There has been a marked improvement in understanding specific processes in catalysis over the past five years. This new fundamental knowledge has provided the basis for advances in alkane (C-H) activation, selective upgrading of methane via selective oxidation, new routes to value-added chemicals through selective oxidation of hydrocarbons, polymerization catalysis, CO and CO_2 conversion, and new catalyst concepts for emissions control which will perform under "lean burn" conditions, as required for advanced gasoline and diesel engines.

- Basic research on single site metalocene catalysts has enabled the development of a revolutionary new process for the industrial scale production of a new generation of polyolefin polymers with superior performance characteristics. The remarkable stereospecificity features of these new catalysts have led to a variety of new, advanced polymer products over a wide range of densities.

- A new nano-phase graphitic material capable of absorbing as much as three grams of hydrogen for each gram of carbon has been discovered by researchers studying catalyst deactivation. The discovery has high potential significance to hydrogen storage technology, and perhaps also to storage of other small gases.

- Fundamental studies on metal-catalyzed polymerizations have led to new materials applications. For example, a palladium-based catalytic system generates polyketone polymers used in gears for business machines, liners for flexible fuel hoses, and industrial molded parts. In another case, a low-cost, catalytic route for the manufacture of advanced polymer materials, namely, polyoxalate polymer resins, are now under study for use in making bioabsorbable sutures.

Portfolio Summary

This portfolio area, "Efficient Energy Use," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activities that strongly support or moderately support Efficiency Energy Use, including combustion-related sciences, advanced materials, engineering sciences, and catalysis and chemical transformations. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

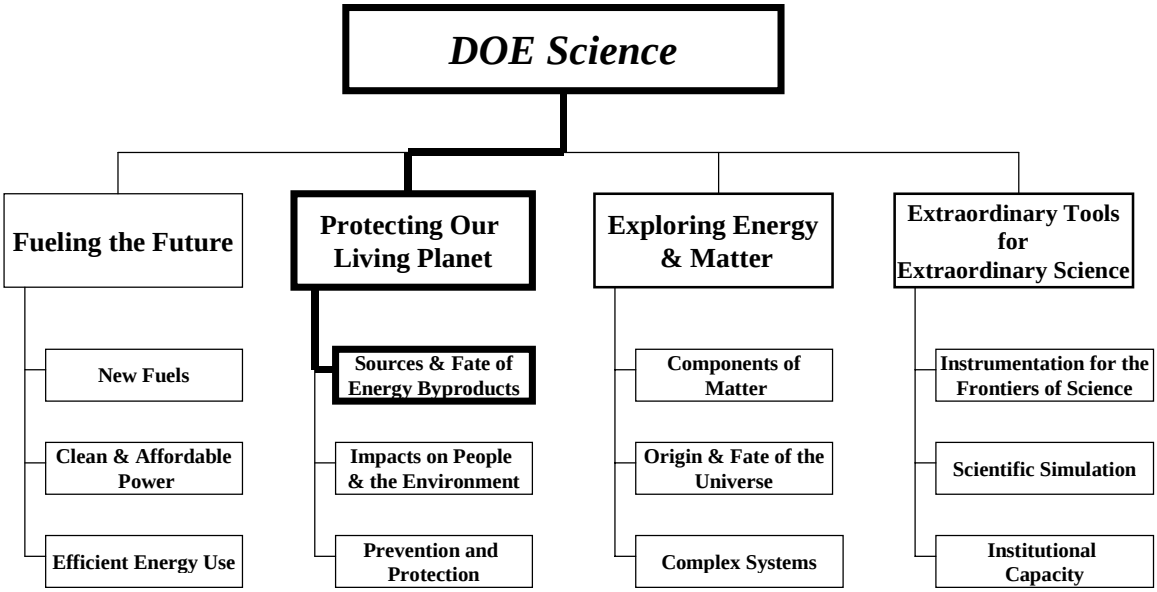
Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations
Advanced Computing Software and Collaboratory Tools
Catalysis and Chemical Transformations
Chemical Physics Research
Engineering Behavior
Laboratory Technology Research and Advanced Energy Projects
Mechanical Behavior and Radiation Effects
Mechanical Systems, Systems Science, and Engineering Analysis
Physical Behavior of Materials
Scientific Computing Application Testbeds
Structure of Materials

Moderately Supportive Core Research Activities
Chemical Energy and Chemical Engineering
Computer Science to Enable Scientific Computing
Environmental and Molecular Sciences Laboratory (EMSL)
Experimental Condensed Matter Physics
Experimental Program to Stimulate Competitive Research (EPSCoR)
General Purpose Plant & Equipment (GPP/GPE)
High Performance Computer Networks
Materials Chemistry
Multiprogram Energy Lab Facilities Support (MELFS)
Neutron and Light Sources Facilities
Neutron and X-Ray Scattering
Oak Ridge Landlord
Photochemistry and Radiation Research
Science Education Support
Separations and Analysis
Small Business Innovation Research (SBIR) Program
Small Business Technology Transfer (STTR) Program
Theory & Simulations of Matter, Engineering Physics

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 5
Sources and Fate of Energy Byproducts

Scientific Challenge: ***To understand the molecular, atmospheric, geological, and biological pathways of energy byproducts in the biosphere.***



Chapter 5

Sources and Fate of Energy Byproducts

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In the years following World War II, it became clear that concerns over the health impacts of released radioactivity depended not only on epidemiology and radiation biology, but also on knowing the fate of airborne radioisotopes. Meteorology and oceanography were no less important than biology, as was research into the ecological processes that cycled materials through plants and animals to human beings. Atmospheric and environmental studies thus became a part of the responsibilities of the Atomic Energy Commission (AEC). These early studies led the AEC and later ERDA (the Energy Research and Development Agency) to initiate environmental and ecological research and global change research programs in the United States.

Today, DOE is seeking to better understand the environmental fate of energy and defense byproducts. The transport, behavior, and fate of byproducts, such as greenhouse gases, local air pollutants (SO_x, NO_x, particulates), and other contaminants must be understood to provide a scientific basis for predicting and prioritizing, and for developing realistic standards. We need to understand how energy-related byproducts move through the biosphere. Subsurface microbial communities alter the chemistry of these byproducts, influence their transport, and offer hope to facilitate remediation of subsurface contaminants. This knowledge will improve our understanding of the feedbacks and interactions among various processes and cycles in the environment, leading to an improved predictive framework to support risk assessment and policy decisions.

Sources and Transport in the Biosphere

Description, Objectives, and Research Performers

Research is conducted on fundamental geological, atmospheric, and biological processes responsible for transporting, concentrating, and localizing energy byproducts in the subsurface, the atmosphere, oceans, and the terrestrial environment. A key component is the development and use of state-of-the-art instrumentation and facilities needed to understand these processes. Emphasis is placed on understanding atmospheric processes that affect air quality and climate change, and on determining the mechanisms that regulate the balance of carbon between the atmosphere, and terrestrial and aquatic ecosystems. Research in this area is conducted at national and other government laboratories, universities and, to a lesser extent, industrial firms.

Research Challenges and Opportunities

A major uncertainty of the greenhouse gas and potential climate change issue is what happens to the excess carbon dioxide (CO_2) generated from the burning of fossil fuels. The amount of CO_2 that remains in the atmosphere is determined by the amount assimilated by the terrestrial and oceanic environment. Assimilation is controlled in large measure by biological processes. Understanding the biophysical mechanisms of the carbon cycle —from the molecular to the ecosystem scale—provides the scientific foundation for estimating capacities and location of carbon sequestration by terrestrial ecosystems and ocean biology. There are also major scientific uncertainties in the behavior of local air pollutants (SO_x, NO_x, particulates) and radionuclides, metals and other chemical contaminants in the atmosphere and the subsurface. Research to understand complex physical, chemical, and biochemical reactions undergone by contaminants in the subsurface and the atmosphere is needed to better understand and predict their behavior and effects.

Research Activities

AmeriFlux experiments measure CO_2 fluxes at sites across North America to estimate carbon sequestration by terrestrial ecosystems. Scientists are developing analytical chemistry techniques, including sensors, for radiation and chemical monitoring. Through this, researchers are characterizing basic chemical, physical, geological, and biological processes affecting contaminant transport in the biosphere. Emphasis is placed on studies of tropospheric ozone and particulate matter to better characterize and predict air quality. Characterization of microbial communities in coastal and subsurface environments aids in understanding the role of microbes in the cycling of carbon and nitrogen and the behavior of other energy byproducts.

Accomplishments

- Research has shown that forested ecosystems represent a significant sink for carbon dioxide sequestration. New data from the Ameriflux network of research sites show that carbon uptake by forests increases with increasing temperature along a climate gradient in eastern North America. These observations are key to our understanding of natural carbon cycles, including the potential effects of climate change on carbon sequestration by forest ecosystems.

- A method has been developed to assess the reactivity of some site contaminants at Idaho National Engineering and Environmental Laboratory (INEEL) with basalt rock formations. This method, based on secondary ion mass spectrometry, could guide the development of cleanup strategies for certain classes of contaminants.

- New methods for sensing and predicting fractures and failures in stressed rock improve our ability to predict contaminant pathways, a critical capability for monitoring and predicting the stability or movement of subsurface contaminants.

- An air chemistry study in the Phoenix area, conducted in collaboration with the Arizona Department of Environmental Quality, indicates that photochemical processing of vehicular nitrogen and hydrocarbon emissions accounts for most of the ozone production in the Phoenix area, but that long-range transport of airborne chemicals from the south also contribute to ozone in the lower atmosphere in the area. Results also show that biogenic hydrocarbons have virtually no role in ozone formation in Phoenix, and that the rate of ozone fomation in Phoenix is much slower than in the eastern U.S. because of lower water vapor concentrations in the atmosphere.

Chemical Interactions and Transformations

Description, Objectives, and Research Performers

Research is conducted on fundamental mechanisms and pathways for biotransformation and biodegradation of contaminant mixtures and for chemical reactions and interactions of energy byproducts in the subsurface and the atmosphere. Research is primarily conducted at national laboratories and universities.

Research Challenges and Opportunities

There are major uncertainties in the reactivity and transformations of atmospheric constituents and pollutants, requiring both laboratory and field studies of atmospheric chemistry and behavior. While, the degradation of many organics and the biotransformation of some inorganic compounds in laboratory cultures have been well described, it is unclear how this information relates to the degradation and transformation of these materials in the environment. Scientists need to understand biotransformation processes such as metal biotransformations and biosequestration, coupled aerobic and anaerobic processes, co-metabolism, biotransformations in the presence of alternative electron donors/acceptors, and biotransformations catalyzed by consortia of microbes. Also needed is understanding of the mechanisms of action and the development of catalysts that are or could be used to transform energy byproducts such as carbon dioxide. There are also significant opportunities to understand the chemical and physical behavior of contaminants, such as actinides, in complex media such as the subsurface. This knowledge will assist the cleanup effort at former defense sites and contaminated industrial sites, and help to calibrate atmospheric models' responses to future pollution levels. In addition, there are major challenges in understanding the role of atmospheric aerosols with regard to air quality, climate change, and human health. A new Tropospheric Aerosol Program is being developed to provide a much more complete understanding of the processes governing the loadings, composition, and microphysical properties of atmospheric aerosols.

Research Activities

Studies are underway to determine the mechanisms and potential of microbes and microbial consortia to biotransform, biodegrade, and sequester energy byproducts such as plutonium, uranium, actinides, chromium, lead, and organic solvents. Research in the chemistry of photochemical oxidants and atmospheric aerosols is being conducted to improve atmospheric models that predict the atmosphere's response to future levels of pollutants. Basic research on actinide chemistry is also emphasized because of the importance of these elements to nuclear and medical technologies and to aid in the remediation of former weapons production sites. Research in the chemistry of photochemical oxidants and atmospheric aerosols is being conducted to improve atmospheric models that predict the atmosphere's response to future levels of pollutants and to provide a sound scientitific basis for strategies and policies intended to protect and enhance air quality.

Accomplishments

- Microorganisms capable of reducing uranium and technetium were isolated from a Uranium Mill Tailings Remedial Action (UMTRA) site. This demonstrates the potential to use bioremediation to remove these radioactive contaminants in the groundwater and subsurface sediments at these UMTRA sites by stimulating the naturally-occurring bioremedation capacity of the microorganisms to form precipitates and immobilize the contaminants in situ.

- Critical information about interactions of chromium and a common soil bacterium were identified, including a map of the spatial distribution and the chemical speciation of the toxic metal, Chromium (VI) were obtained using the Advanced Photon Source.

- New instruments were developed and installed in the field to characterize aerosols in the atmosphere, including the size distribution and number density of fine particles with diameters from 3 nanometers to 3 micrometers in size, the composition of individual ambient aerosol particles, and the composition of inorganic aerosols on a continuous basis with a time resolution of 5 minutes.

- Laboratory and field studies indicate that the ambient relative humidity and organic content of fine particles in the atmosphere can have a controlling effect on particle-gas interactions as they affect oxidant concentrations in the lower atmosphere.

- Long-term research on heavy metals resulted in metal separation and purification technologies that resulted in the isolation of yttrium-90 from nuclear waste for subsequent use in cancer treatment.

Portfolio Summary

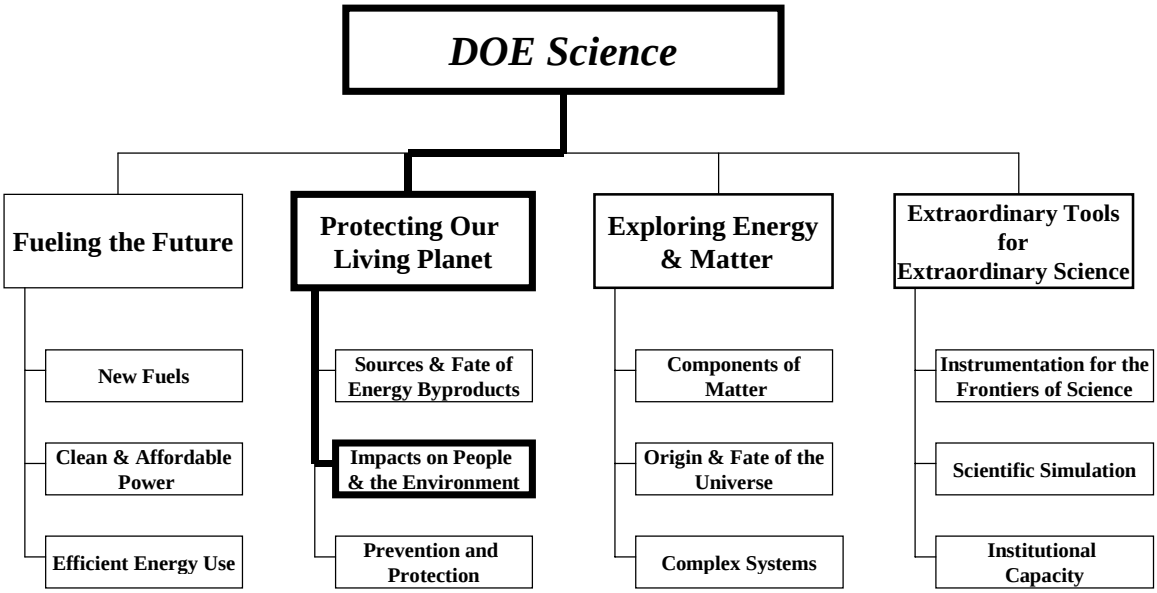
This portfolio area, "Sources and Fate of Energy Byproducts," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activities that strongly support or moderately support Sources and Fate of Energy Byproducts, including sources and transport in the biosphere, and chemical interactions and transformations. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities Analytical Chemistry Instrumentation Atmospheric Radiation Measurement (ARM) Program Infrastructure Atmospheric Radiation Measurement (ARM) Program Research Atmospheric Sciences Carbon Cycle Research Cleanup Research Climate Change Prediction Program Climate Change Technology Initiative (CCTI) Geosciences Heavy Element Chemistry
Moderately Supportive Core Research Activities Catalysis and Chemical Transformations Economics of Global Climate Energy Biosciences Experimental Program to Stimulate Competitive Research (EPSCoR) General Purpose Plant & Equipment (GPP/GPE) Laboratory Technology Research and Advanced Energy Projects Multiprogram Energy Lab Facilities Support (MELFS) Neutron and Light Sources Facilities

Oak Ridge Landlord Photochemistry and Radiation Research Science Education Support Separations and Analysis Small Business Innovation Research (SBIR) Program Small Business Technology Transfer (STTR) Program
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 6
Impacts on People and the Environment

Scientific Challenge: ***To understand and evaluate the effects of energy byproducts on people and the biosphere.***



Chapter 6

Impacts on People and the Environment

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By the time of the Manhattan Project, physicists had almost a half-century of experience with radioactive elements and associated radiation. Several such elements, most notably radium, had been used since the turn of the century in efforts to treat human disease. At the same time, even the earliest scientific pioneers saw that radioactivity was not a benign blessing and that protection standards were necessary. However, it was World War II that demonstrated the atom's incredible power. While the initial focus was on the promise of nuclear energy, a new era had also arrived for biology, medicine, and environmental research.

Even during the war years, biological research was a priority. Among the ongoing efforts were health physics research for improving our knowledge of the potential dangers presented by fissionable materials, reactors, and fission products, and for proposing methods of identifying or avoiding such dangers.

Even the Human Genome Project is a surprising but logical offspring of longstanding research on health issues and genetic effects, research that is or will be the underpinning of radiation protection standards today and in the future.

Energy byproducts also interact with and have impacts on the environment. In addition to characterizing, measuring, and predicting events at the molecular level, scientists must understand their interactions for regional and global scale phenomena. A predictive understanding of relations between energy use and environmental response, including the complex interaction of the ocean, atmosphere, and land system, is required to support decisions in the energy, environment, and economic policy arena. Key to this effort are sophisticated computer models that take into account the physical, chemical, and biological processes involved. A broad spectrum of models is being developed, validated, and employed to predict long-term trends in climate and related environmental systems down to the regional level.

Human Health Impacts and Risks

Description, Objectives, and Research Performers

The Department has a broad base of information on the health effects of exposures to high doses of radiation; however, several recent studies suggest that tissues and whole animals respond to toxic substances differently at high and low doses. Thus, current research on the health effects of low-dose or low-dose-rate exposures to radiation builds on these previous studies and takes advantage of new knowledge and tools gained from the Department's human genome and structural biology research. The goal is to ascertain the health effects, from cells to whole organisms, from low-dose-rate exposures to energy and defense-related insults to ionizing radiation. This program will provide information that will decrease the uncertainty of risk at low levels, help determine the shape of the dose-response relationships after low level exposure, and achieve acceptable levels of human health protection at the lowest possible cost. Research is currently conducted at national laboratories and universities, and, to a lesser extent, other government laboratories.

Research Challenges and Opportunities

Protection of human health is a key driver in developing new energy technologies, in manufacturing, and in cleaning up contaminants from previous energy-related activities. Scientists need to determine what levels of exposure to chemicals and radiation would be consistent with achieving acceptable protection of human health. Current standards for occupational and residential exposures to radiation and chemicals are based on linear, no-threshold models that assume risk is always proportional to dose, i.e., there is no risk only when there is no dose. However, the scientific basis for these assumptions is limited and uncertain at very low doses. Much evidence suggests that the risks from exposure to low doses of radiation and chemicals may be better described by a nonlinear, dose-response relationship.

Research Activities

The program includes research to identify and characterize (1) differences or similarities between the biological damage from and responses to low doses of radiation versus normal oxidative processes in cells; (2) whether there are thresholds for low dose radiation; (3) genetic factors that affect individual sensitivity to and risk from radiation; and (4) how we communicate research results.

Accomplishments

This new research program issued its first solicitation in FY 1998. It is built on over 50 years of DOE research on the health effects of radiation and chemicals, primarily conducted at high doses. Significant (past) accomplishments that underpin this new research program include:

- A mouse assay, still in use today, was developed for assessing the risks to humans from exposure to radiation and chemicals.
- Researchers discovered DNA repair and the ability of most organisms to repair radiation and chemical damage. The DNA repair molecule was named molecule of the year by *Science* magazine in 1995.
- Researchers demonstrated that a human disease associated with susceptibility to cancer is caused by a genetically impaired ability to repair damaged DNA.
- A bacterial assay, known as the Ames test, was developed and is widely used by government and industry to identify potential cancer-causing chemicals or pharmaceuticals.
- The Human Genome Project has revolutionized the entire field of biology and spawned the biotechnology industry. It was initiated by the Department to develop biological information and tools needed to determine and understand the genetic effects of human exposures to low levels of radiation and chemicals.
- Researchers demonstrated that the microenvironment of tissues contains adhesion molecules that regulate gene expression.

Ecosystem Responses

Description, Objectives, and Research Performers

Research is conducted to understand responses of terrestrial ecosystems and organisms to changes in climate and atmospheric composition, such as temperature, moisture, and CO_2. This research will improve our understanding of (1) how terrestrial organisms and ecosystems respond to simultaneous changes in the composition of the atmosphere and in climate, (2) the biological or ecological mechanisms or pathways leading to those responses, and (3) the extent to which the responses are seen across different levels of the terrestrial ecosystem that affect humans positively or negatively. Research is conducted primarily at national laboratories and universities.

Research Challenges and Opportunities

Knowledge of possible effects of climate and atmospheric changes on ecological systems has increased over the past decade and qualitative estimates of responses to such changes can now be developed. However, scientists are still unable to make accurate quantitative predictions of the effects of changes in climate and atmospheric composition on ecosystems. A better understanding is needed of many critical processes such as the effects of climate changes and increasing atmospheric CO_2 on particular ecosystems at particular locations or regions. Researchers need to understand the climatic and non-climatic factors that influence the structure and functioning of terrestrial ecosystems. Research is also needed on the dynamic responses of ecosystems to simultaneous changes in multiple factors, particularly human-induced changes to which the ecosystems have not been previously subjected.

Research Activities

Experimental and modeling studies on different types of ecosystems investigate system responses to alterations in climate variables, atmospheric CO_2, ozone, and nutrient inputs. Two examples of this research are the Free Air CO_2 Enrichment Experiments (FACE) and the Throughfall Displacement Experiment. FACE research evaluates the responses of terrestrial plants and ecosystems, including forest, grassland, desert, and croplands, to known (increased) concentrations of atmospheric CO_2 and altered temperature and precipitation regimes. A Throughfall Displacement Experiment studies the response of a forest ecosystem to changing precipitation inputs. These studies document ecosystem responses, including changes in physiological processes, above- and below-ground growth responses, and other functional and structural responses of the experimental and control ecosystems being studied. Results will be used to develop and apply ecosystem response models that are intended to assess the consequences of human-induced environmental changes on terrestrial ecosystems.

Accomplishments

- Seven long-term experiments were initiated on the physiological and growth responses of forest, grassland and crop species, and ecosystems to variations in climate such as CO_2, temperature, and precipitation. These experiments will determine whether or not altered growth responses to elevated atmospheric carbon dioxide are sustained, how the systems

respond to interannual variation in other environmental factors, including climate, and if changes in competitive interactions between species occur for limited resources that lead to different responses between species over time.

- Initial results from long-term FACE experiments show that increased CO_2 caused greater productivity and improved water use efficiency of these systems. A significant part of the productivity increase occurs below ground, involving roots, soil micro flora and the formation of soil organic matter.

- Findings from the Throughfall Displacement Experiment after six years show that changes in the seasonal timing of rainfall has a greater effect on the productivity of forest ecosystems and carbon sequestration by forests than a uniform change in rainfall applied throughout the year. Initial results of a factorial FACE experiment designed to measure the response of regenerating forests containing aspen, sugar maple and birch trees exposed to elevated carbon dioxide, elevated ozone, and elevated CO_2 plus ozone show that second-year growth of aspen and birch is increased by elevated CO_2 and decreased by elevated ozone and elevated CO_2 plus ozone compared to the controls. Insect populations, including species considered to be pest species in forests, have increased in the stands exposed to elevated CO_2, elevated ozone, and elevated CO_2 plus ozone compared to the controls, suggesting that the chemistry of trees in these treatments has been altered in a way that attracts more insects.

Regional and Global Consequences

Description, Objectives, and Research Performers

The Climate Change Prediction Program develops models that predict future climate given present and projected modifications such as changes in greenhouse gases. Efforts include increasing computational capabilities, the speed of computations, and the resolution and validity of the models. The models feed into a national effort coordinated with other agencies, including the National Science Foundation at the National Center for Atmospheric Research (NCAR). The Department's efforts have a primary focus on decade-to-century climate simulations. Capability to accurately simulate climate is currently limited by lack of understanding and modeling of the effects of clouds in climate. The Atmospheric Radiation Measurement Program (ARM) uses heavily instrumented sites and long-term observations to provide data and modeling improvements for climate prediction. Models are also developed for terrestrial carbon processes that, when coupled with atmosphere-ocean carbon models, estimate the rate and timing of atmospheric CO_2 change. Information from modeling efforts is integrated into efforts to assess the costs and impacts of potential changes in climate, including potential actions to ameliorate climate change. Research is conducted at national laboratories, universities, industrial firms, other government laboratories, and, to a minor extent, internationally.

Research Challenges and Opportunities

The most obvious challenge in climate change prediction is the increase in resolution required to achieve the regional scale simulations needed for meaningful assessments of the impacts of climate change. Increases in resolution require new models for meteorological phenomena

because of differences in the scales of different phenomena. The role of clouds in climate prediction limits both global and regional predictive capability. Research to develop adequate models for cloud reflectivity and absorption is being pursued through extensive data gathering and intensive analysis and comparison of data with models. Development of effective cloud models for climate prediction will enable global and regional climate prediction over both the shorter and decade-to-century time spans. An understanding of climate variability is needed to address long term energy needs and usage impacts. A major uncertainty linking greenhouse gases and climate change is the fate of the excess CO_2 generated when fossil fuels are burned. The amount of CO_2 that remains in the atmosphere is determined by the amount taken up by terrestrial and oceanic sinks, which in turn is largely controlled by biological processes. Scientists need to understand the biophysical mechanisms of the carbon cycle to estimate capacities and locate carbon sequestration by terrestrial ecosystems and ocean biology. The effects of non-CO_2 greenhouse gases, many of them also byproducts of energy use, also need to be represented as part of integrated models to assess potential impacts of climate change.

Research Activities

The Atmospheric Radiation Measurement (ARM) Program (1) develops instruments and maintains field research sites to collect data on clouds and their role in reflecting and trapping both solar (incoming) and infrared (outgoing) atmospheric radiation and (2) collects and analyzes data for use in General Circulation Models (GCMs), the primary tool with which climate predictions are made. The Climate Change Prediction Program develops algorithms for climate modeling efforts on massively parallel computers, develops models for climate effects such as the effects of plant activity on the hydrologic cycle, develops components of major ocean and atmospheric models, and compares the output of models with data and observed phenomena. Data is collected as part of the AmeriFlux network and FACE for use in modeling the carbon cycle.

Accomplishments

- A Parallel Climate Model, developed at Los Alamos National Laboratory in collaboration with the Naval Postgraduate School to understand and predict the role of the oceans in global climate change, was successfully incorporated into the suite of models used by the National Center for Atmospheric Research to predict future climate. This model will be used by much of the scientific community in the next few years.

- An improved radiation transfer model developed by the ARM Program has been implemented in the European Center for Medium-Range Weather Forecasts (ECMWF) model used to predict weather.

- An improved cloud model was developed for the NCAR Climate System Model

- A Millimeter Cloud Radar at the ARM Southern Great Plains site is providing continuous data to improve cloud characterization and modeling.

- The first three-dimensional quantified distribution of clouds, cloud water, and cloud ice was acquired. These data will allow better representation of clouds in climate models.

- Integrated assessment models are used by decision makers and advisory bodies such as the Council of Economic Advisors to assess potential environmental and economic costs and benefits of alternative energy and pollution mitigation policies and strategies.

Portfolio Summary

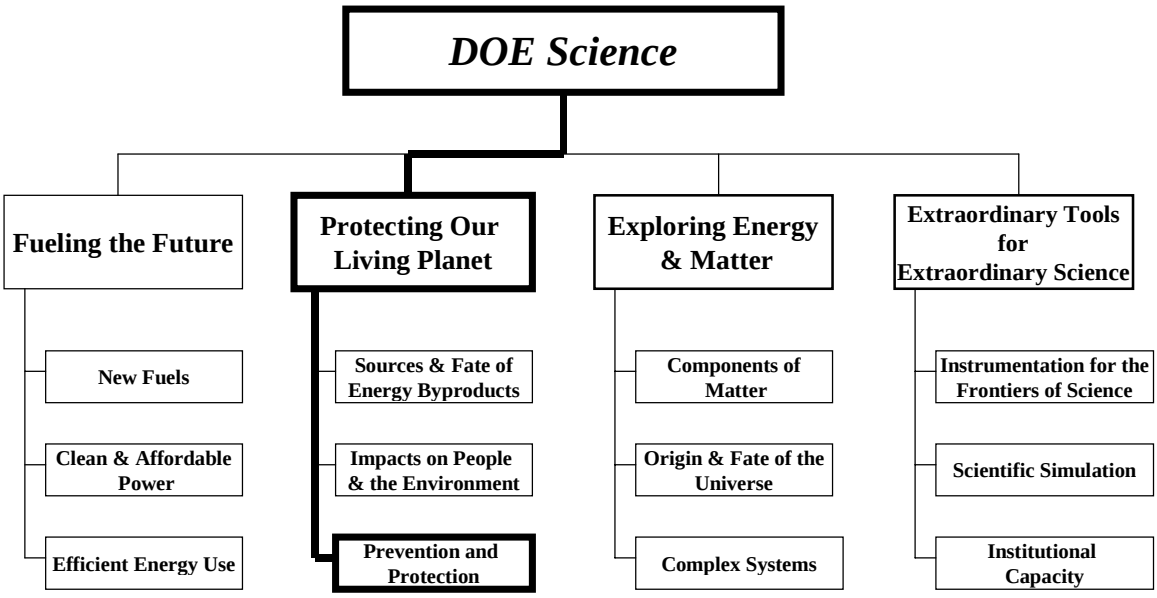
This portfolio area, "Impacts on People and the Environment," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activities that strongly support or moderately support Impacts on People and the Environment, including human health impacts and risks, ecosystem responses, and regional and global consequences. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations Atmospheric Radiation Measurement (ARM) Program Infrastructure Atmospheric Radiation Measurement (ARM) Program Research Atmospheric Sciences Carbon Cycle Research Climate Change Prediction Program Climate Change Technology Initiative (CCTI) Ecological Processes Economics of Global Climate Environmental and Molecular Sciences Laboratory (EMSL) Health Risks from Low Dose Exposures Natural and Accelerated Bioremediation Research Program
Moderately Supportive Core Research Activities
Advanced Fusion Design Advanced Fusion Materials Research Advanced Medical Imaging Cleanup Research Computer Science to Enable Scientific Computing Energy Biosciences Focused Health Research Fusion Technologies General Purpose Plant & Equipment (GPP/GPE) Laboratory Technology Research and Advanced Energy Projects Microbial Genomics Multiprogram Energy Lab Facilities Support (MELFS) Oak Ridge Landlord Science Education Support Small Business Innovation Research (SBIR) Program

Small Business Technology Transfer (STTR) Program
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 7
Prevention and Protection

Scientific Challenge: ***To create new scientific approaches to protect the biosphere from the effects of energy byproducts.***



Chapter 7
Prevention and Protection

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A technological revolution is underway that will impact America's most important industries, including agriculture, chemicals, medicine, and energy production. The Department's research in genetic and biomolecular structure and in computational biology is initiating this revolution. In the future, the nation will have truly remarkable technological capabilities at its command. Energy production from fossil and renewable resources will have higher yields and generate negligible environmental pollution. New varieties of plants will be developed for renewable biomass-based energy production using our knowledge of the genetic code. New biomolecules designed for efficient energy production, environmental cleanup, and management of atmospheric carbon will have been created using design methods similar to those currently used in the manufacture of industrial components.

These advances will all stem from new knowledge of the molecular nature of life and of materials. In particular, they will arise from our increasing knowledge of the relationships between macromolecular structure and function, and from our ability to modify structure to create particular functions or properties in macromolecules.

When the veil of wartime secrecy was lifted from the nuclear reactor at the Clinton Laboratories (now Oak Ridge National Laboratory) in 1946, the Atomic Energy Commission (AEC) inherited a developing field of nuclear medicine full of potential. New radioisotopes—iodine-131, technetium-99m, carbon-14, thallium-201, and gallium-67, to name a few—were produced for the biomedical community. Their impacts on diagnosis and therapy have been enormous. In 1995, nearly one million thallium-201 heart scans were performed in the United States alone. About 13 million patients per year, roughly one-quarter of all U.S. inpatients, receive technetium-99m scans. But the diagnostic value of radioisotopes could only be realized with the simultaneous development of corresponding imaging devices. Simple imaging devices gave way to devices that produced images in three dimensions. AEC research laid the foundation for the development of widely used CT (computed tomography) and PET (positron emission tomography) scanners. Today, imaging technology is central not only to medical diagnosis but also to understanding organ function and dysfunction.

Pollution Minimization

Description, Objectives, and Research Performers

A broad range of pollution minimization research is supported that impacts energy production and use. The DNA sequence and functional capabilities of microbes that produce methane or hydrogen, for example, are characterized. This information, coupled with structural and computational biology research, provides opportunities for the use and redesign of microbes for energy uses. Engineering research is conducted on combustion and fuel bioprocessing for more efficient fuel use and waste minimization. Research on non-automotive battery systems improves battery size, weight, life, and recharge cycles. Research is conducted primarily at national and other government laboratories and universities and, to a lesser extent, industrial firms.

Research Challenges and Opportunities

Microbes make up approximately 60% of the earth’s biomass. They have survived on earth for over 3.7 billion years and are found surviving extremes of heat, cold, radiation, pressure, salt,

and acid. An important scientific challenge is to identify microbes and microbial capabilities that already hold solutions to important problems, such as efficient energy production, environmental cleanup, and management of atmospheric carbon.

High throughput structural biology and computational approaches are needed that can better keep pace with advances in DNA sequencing ability, and to determine the structure and function of large numbers of useful proteins. The resultant biological information, coupled with a better understanding of the engineering and use of nanoscale systems can deliver powerful new solutions for producing and using energy with minimal pollution.

In order to achieve higher energy yields and negligible environmental pollution, researchers are challenged to develop and refine combustion models used to predict the efficiency and emission characteristics of combustion devices and to optimize and control combustion processes.

Research Activities

The DNA sequences of energy-related microbes are determined and annotated to identify all the potential genes encoded in their DNA and to get clues about their potential functions. Structural information is determined on selected proteins from these microbes. Research is conducted on combustion-related chemical physics and in the fundamental chemical engineering sciences underpinning energy intensive chemical processes including electrochemical storage and conversion and turbulence in combustion.

Accomplishments

- The complete genome of 11 microbial species have been sequenced and published and 15 more are in various states of sequencing. The availability of information on the complete DNA sequence of these microbes provides opportunities for the development of new tools to remediate contaminated environments, new energy sources, therapeutic and diagnostic resources for medicines, and important industrial products.

- The DNA sequences of several energy-related microbes have been or are being determined to provide information needed to develop new or improved energy sources that minimize pollution. The microbes being characterized include *Archaeoglobus fulgidus* (active in oil well souring), *Thermotoga maritima* (used for energy generation from biomass), *Methanobacterium thermoautotrophicum* (a methane producer), and *Carboxydothermus hydrogenoformans* (a hydrogen producer).

- The DNA sequence of Chlorobium tepidum, a microbe considered to be a major player in global carbon management and whose DNA sequence is an important first step for developing new strategies to reduce excess carbon in the atmosphere, was determined.

- A simple, elegant experiment demonstrated an error in current models for basic combustion processes. This new knowledge will accelerate our ability to understand and control combustion.

- Basic science research has led to the development of current generation high energy and power lithium and lithium ion batteries, improvements in the safety of rechargeable batteries, and thin film lithium batteries half the thickness of household plastic wrap.

Cleanup and Remediation

Description, Objectives, and Research Performers

Natural and Accelerated Bioremediation Research (NABIR) provides fundamental science that serves as the basis for developing cost-effective bioremediation of radionuclides and metals in the subsurface at DOE sites; understanding intrinsic bioremediation and opportunities for accelerated bioremediation using chemical and microbial amendments; integrating bioremediation with conventional physical-chemical remediation to accelerate site cleanup; and evaluation of bioremediation by regulators, local communities, and other stakeholders. NABIR emphasizes characterization and use of microbes and microbial communities with bioremedial potential. The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) operates more than 100 leading-edge computational and research systems as part of a national collaboratory user facility for molecular level environmental research. Research is also supported on fundamental molecular level questions underlying the most energy-consuming industrial process, separations, a key component of environmental cleanup. Research is conducted at national laboratories, universities, and industrial firms.

Research Challenges and Opportunities

Former DOE weapons sites contain complex mixtures of chemicals, metals, and radionuclides that need to be cleaned up. It may be possible to supplement or replace current cleanup strategies with new approaches that will be more efficient and cost effective. Developing these new cleanup strategies requires a wide array of scientific information and technological developments. We need to (1) determine the fate of metals and radionuclides in complex, heterogeneous matrices such as subsurface sediments; (2) scale up research from the laboratory to field scale; (3) communicate research findings to a broad audience such as regulators, site managers, tribes and communities; (4) identify, engineer, and exploit microbes with bioremediation potential; (5) develop improved and novel separation technologies, including ceramic membranes, new materials derived from combinatorial chemistry approaches, and novel separations (based on self-assembly systems, combined separation and reactive systems, tailored inorganic systems, and the use of macromolecules such as dendrimers); and (6) develop and implement ultra-sensitive detection capabilities such as single molecule detectors.

Research Activities

Research studies are underway to determine the DNA sequences of microbes with bioremediation potential and to “annotate” the sequences to identify all potential genes and obtain clues about their potential functions. Scientists are seeking to determine structural information on selected microbial proteins. NABIR projects address the biotransformation of contaminants, microbial community dynamics, biomolecular science and engineering to improve and exploit the bioremedial capabilities of microbes, biogeochemistry, assessment of the effectiveness of bioremediation, acceleration of the natural bioremedial capabilities of native

microbes, and bioremediation-related societal issues and concerns. Research is supported to improve understanding of methods for separating mixtures of gases, liquids, solids, and their component molecules, cations, and anions.

Accomplishments

- Gene transfer systems have been developed for Geobacter sulfurreducens, a metal and radionuclide reducing bacterium that has been found to be present in the subsurface in diverse geographic environments. The complete genome for this bacterium is now being sequenced and this information will provide opportunites to use this organism in developing bioremediation strategies for subsurface environments contaminated with metals and radionuclides.

- Genes for mercury resistance have been cloned into Deinococcus radiodurans, a highly radiation resistant microbe. Utilizing this genetically modified microbe may enable the remediation of mixed wastes containing high levels of both stable mercury and radionuclides that would be chemically and radiologically toxic to other microbes.

- Over 600 scientists used EMSL to carry out cutting-edge environmental and molecular research in its first year of operation.

- A new technetium extraction process has been developed, for potential use in the Hanford waste tanks. This process will significantly reduce the final volume of waste that will require costly processing and long term storage.

- High-resolution images of metal oxidizing and reducing bacteria have been taken, helping to reveal the role of these organisms as potential agents for bacterial bioremediation. High-resolution spectroscopic measurements have revealed the chemical state of pollutants at extremely low concentrations.

- A suite of new bacterial tracking tools has been field tested, with implications for determining the movement and distribution of injected bacteria. Such biochemical tacking tools are critical to enhancing the reliability of bioaugmentation, one type of bioremediation, which has not yet reached its full potential for cleanup of contaminated environments.

Carbon Sequestration

Description, Objectives, and Research Performers

This new program will provide scientific knowledge on biological processes that drive carbon exchange between the oceans and the atmosphere and between the atmosphere and the terrestrial environment. Genomic DNA sequences will be determined for microbes that play a role in the sequestration of carbon in the oceans or the terrestrial biosphere. Options for storing excess carbon in the deep oceans, in subsurface geologic structures, or using biological solutions will be investigated. Research will be conducted at national laboratories, universities, and industrial firms.

Research Challenges and Opportunities

Implementing carbon management on the scale needed to impact global carbon dioxide levels requires new levels of understanding, from the molecular to ecosystem scale, about geological, chemical, physical and biological interactions between carbon and the environment. Completely new approaches to carbon management will be investigated. These approaches will build on scientific breakthroughs in molecular design or genetic engineering of plants and microorganisms and on advances in understanding of the complex chemical and physical interactions that occur with subsurface geologic structures and aquifers. New techniques to monitor biogeochemical processes and ecosystem impacts of changes in the carbon cycle will be developed to anticipate and assess the environmental impacts associated with various biological and physical approaches to carbon sequestration.

Research Activities

This new research program issued its first solicitations for research proposals in FY 1999. Biological research will focus on carbon sequestration in terrestrial ecosystems and the ocean, including both natural and managed ecosystems. Impacts of alterations in the carbon cycle on other elemental cycles, such as nitrogen, will be determined. Microbial genome research will identify and characterize (including genomic DNA sequencing) microbes that play a role in natural carbon cycles to develop novel strategies and tools for manipulating and modeling entire biochemical reaction pathways or regulatory networks that could be used to increase their role in carbon sequestration. Photosynthesis research will focus on understanding and characterizing the genes and regulatory mechanisms involved in photosynthetic fixation of carbon and the subsequent metabolism of fixed carbon. Research may lead to new strategies for replacing fossil fuels with biologically fixed carbon, including fuels and chemical feedstocks, and for altering steady-state levels of atmospheric CO_2. The potential for deep underground sequestration of carbon will lead to research that addresses (1) geometric, structural, and hydrological reservoir descriptions of potential storage sites, (2) changes in reservoir characteristics with drilling and fluid injection, and (3) the physics of multiphase flow in fractured rock systems. Finally, the potential ecological impacts of various carbon sequestration strategies will be evaluated.

Accomplishments

- Two Laboratory Centers for carbon sequestration were created; one focusing on mechanisms of sequestration in terrestrial ecosystems and the second focusing carbon sequestration in the ocean, including the potential impacts of enhanced carbon sequestration or disposal in the ocean. The centers are actively engaged in cooperative programs with a number of academic and private research institutions and other agencies and the approach is to explore opportunities for enhancing natural processes of carbon sequestration and improving understanding of the environmental implications of enhancing the sequestration.

- Genomic DNA sequencing of four carbon sequesteration-related microbes, including Nitrosomonas europeae, Prochlorococcus marinus, Rhodopseudomonas palustris, and Nostoc spp. -- have been selected for genome sequencing and are in various stages of completion.

- The basic biophysics and biochemistry of photosynthetic energy capture and of the photosynthetic apparatus have been characterized.
- Scientists have improved understanding of basic mineral-fluid interactions important for developing strategies to sequester carbon in geologic structures.
- Advances in geophysical imaging needed to understand subsurface structures and properties have been made.
- Methods were developed to evaluate natural and human-perturbed process in the geologic environment.
- Direct measurements of net carbon sequestration by forest ecosystems demonstrate that both aggrading, second-growth forests and old-growth forests in temperate regions of the U.S. are net sinks for atmospheric carbon dioxide. Information on the biophysical processes controlling the net uptake of carbon in these systems may lead to approaches to enhance the sequestration and retain more of it in these ecosystems systems once it is sequestered.

Health Protection—Regulation and Medicine

Description, Objectives, and Research Performers

Human health is protected through better understanding of health risks from low-level radiation and from improvements in medicine. New information is needed by regulatory agencies to decrease uncertainty of determining health risks from low-level radiation exposures, to help determine the shape of the dose-response relationships after low level exposure, and to achieve acceptable levels of human health protection at the lowest possible cost. Radiolabeled molecules are developed for noninvasive studies of metabolic and physiological processes and for the diagnosis and treatment of disease. New, sensitive, high-resolution positron emission tomography (PET) instruments for radiotraacer imaging and magnetoencephalography (MEG) for probing the tiny magnetic fields in the brain are being developed. Medical applications of lasers are also emphasized. New imaging technology will be used to “see” genes in action, as a molecular monitor for vital organ function, and to monitor the effects of chemo-, radio- and gene-therapy. A new Biomedical Engineering research program has been initiated that includes research on tissue engineering, molecular biosensors, medical imaging, virtual reality, robotics and micromachines, and biomaterials. Compounds are being developed for boron neutron capture therapy (BNCT), a cancer treatment based on the interaction of boron-containing compounds with thermal neutrons that can theoretically kill cancer cells without affecting surrounding normal cellsResearch is conducted at national laboratories, universities, and government laboratories.

Research Challenges and Opportunities

New radiotracer tools are needed to identify steps in gene expression pathways that may be altered in disease states. New molecular markers for specific biochemical phenotypes are needed as targets for molecular-based treatment of cancer and degenerative brain disorders. Rapid

progress in the human genome program and in the development and screening of libraries of new chemical compounds can be used to improve the design and synthesis of new radiotracers that are directed to specific molecular targets. There are significant opportunities to improve imaging detector technology and algorithms used for information processing that will improve spatial resolution, quantitative accuracy, and detection efficiency of medical imaging. The use of these techniques will be expanded from clinical uses in humans to valuable experimental studies in animals. A challenge for biomedical engineering research is to produce new technologies that will have significant impacts on medical care. New classes of boron compounds that selectively accumulate in cancer cells compared to surrounding normal cells are needed for BNCT. Phase I/II BNCT clinical trials need to be completed to unambiguously assess toxicity and effectiveness.

Research Activities

Researchers seek to identify and characterize genes and gene products that determine cellular responses to low doses of radiation and that affect individual susceptibility to low dose exposures. This allows development of methods to incorporate molecular-level information into the estimation of overall health risk. New synthetic organic chemistry techniques are being developed to rapidly radiolabel a wide variety of molecules for targeting many in vivo sites. New radiolabeled compounds are evaluated in vitro and in vivo. Preclinical evaluations are conducted on radiopharmaceuticals for heart and brain disorders, neurodegenerative diseases, cancer, and for development of new molecular targeted therapies.

Ongoing research includes development of a PET scanner capable of <2 mm resolution. miniature radionuclide imagers for small animal and organ specific imaging, a full-head biomagnetometer for the human brain, medical applications of laser technology, and new technologies for merging PET and magnetic resonance imaging (MRI) for anatomically well-defined images of the body's biology. Pre-clinical development of novel boron-containing compounds is underway, and their pharmacokinetics and bio-distribution are being studied. Clinical trials of BNCT for the treatment of brain cancer and melanoma are underway at MIT/ Beth Israel Deaconess Hospital to evaluate its toxicity and efficacy.

Accomplishments

- Technetium-99m generators for bone scanning and other diagnostic studies are now used in 35,000 clinical procedures a day.
- Fluorine-18-fluorodeoxyglucose is now used with PET for imaging and mapping of the normal and diseased human brain.
- Meta-iodobenzylguanidine is a powerful new radiopharmaceutical used to visualize and treat deadly neuroblastomas in children.
- New carbon-11 and fluorine-18 radiotracers are being used to develop new therapies and to study substance abuse, and neurodegeneration.

- New imaging devices include the world's highest resolution and fastest 3D PET instrument, a small animal and breast-specific imager, and laser-based technology for rapid measurements of enzyme activity in single cells.

- PET and magnetic resonance imaging (MRI) were merged, opening new possibilities in diagnostic imaging.

- The most effective boron-containing compound studied to date, boronophenyl alanine (BPA), has been shown to have a preferential uptake in cancer cells versus normal brain of approximately 3-4 to 1, and is currently being investigated for potential clinical use with humans.

- BNCT phase I/II clinical trials are proceeding with approximately 50 patients to date.

Portfolio Summary

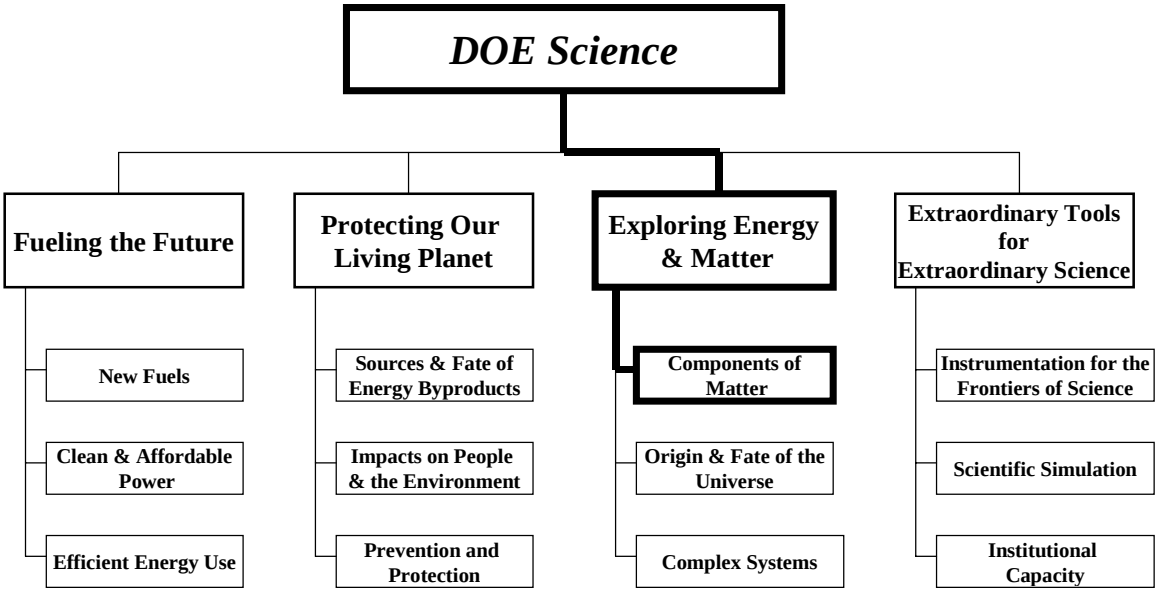
This portfolio area, "Prevention and Protection," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support or moderately support Prevention and Protection, including pollution minimization, cleanup and remediation, carbon sequestration, and health protection. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities Advanced Medical Imaging Analytical Chemistry Instrumentation Boron Neutron Capture Therapy Cleanup Research Climate Change Technology Initiative (CCTI) Environmental and Molecular Sciences Laboratory (EMSL) Laboratory Technology Research and Advanced Energy Projects Microbial Genomics Natural and Accelerated Bioremediation Research Program Radiopharmaceutical Development Science Education Support Separations and Analysis
Moderately Supportive Core Research Activities Chemical Physics Research Energy Biosciences Experimental Program to Stimulate Competitive Research (EPSCoR) Focused Health Research General Purpose Plant & Equipment (GPP/GPE)

Geosciences Health Risks from Low Dose Exposures Heavy Element Chemistry Multiprogram Energy Lab Facilities Support (MELFS) Neutron and Light Sources Facilities Oak Ridge Landlord Small Business Innovation Research (SBIR) Program Small Business Technology Transfer (STTR) Program Structural Biology Research Facilities Understanding and Predicting Protein Structure Understanding Gene Function
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 8
Components of Matter

Scientific Challenge: ***To understand matter at the most fundamental level.***



Chapter 8
Components of Matter

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For more than a century, physical science has been imbued with the "atomistic paradigm," which holds that, at all scales of complexity, from the smallest subnuclear quark to the largest living cell, physical processes can be treated as reactions between the relevant basic units. These units, or "atoms," interact with one another, or combine with one another to form more complex objects, or even occasionally annihilate one another to form pure energy. Each atom, when viewed on its own natural scale, is simple and fundamental, but quickly becomes complex when viewed on a finer scale. Such is the case when we pass from biological molecules, which form the basis of life, down through atoms and nuclei to leptons and quarks, which are the smallest building blocks we have observed up to this time, and which we presently believe to be the fundamental building blocks of all matter. The science portfolio of the DOE Office of Science spans the entire range of scales in the effort to understand the basic properties of matter.

Elementary Particles and Their Interactions

Description, Objectives, and Research Performers

Research into elementary particles and their interactions reflects the quest to uncover the nature of matter at its most fundamental level. With this knowledge, scientists strive to understand why the universe is the way it is. Starting a hundred years ago, the first of the basic particles, the electron, was discovered. So began a remarkable journey inward to smaller and smaller scales, from the atom to the nucleus to the quarks. Much of modern technology is based on the deep understanding of matter that has developed over the last century.

Along with this discovery of the fundamental constituents came a growing understanding of the interactions between them. One of the great achievements of the last quarter century is the understanding that apparently different interactions are unified as different manifestations of a single force. This remarkably simple and beautiful synthesis of ideas regarding the fundamental constituents of matter and their interactions has profoundly changed scientists' thinking about the natural world. Despite this period of great revelation, every turn continues to provide major surprises, forces adjustments in thinking, and spurs scientists' efforts to discover whether all interactions, including gravity, can ultimately be understood in terms of a single theory.

To peer into the microcosm has required great imagination in the design of large, high-energy particle accelerators, the fundamental probe for the journey inward. The seeming paradox exists that to observe the smallest objects requires the most energy—energy almost beyond comprehension—to explore a realm governed by both relativity and quantum mechanics. Yet the technology developed in pursuit of this fundamental knowledge has led to many other remarkable applications, including radiation therapy, neutron sources used for materials science, and synchrotron light sources used for research in many fields, including materials science, environmental chemistry, and structural biology.

Research into elementary particles and their interactions is carried out primarily at universities and, to a lesser extent, at national laboratories. Industry participation is limited to modest funding for research supporting advanced particle accelerator concepts.

Research Challenges and Opportunities

All of the forces discussed in the previous section are characterized by interaction strengths that increase very slowly, but steadily, with the energy of a particular interaction process. Unification of the forces means that at some very high energy, much higher than has been obtained in present-day laboratories, they attain exactly the same strength. There are indications from our present knowledge that the strengths might well extrapolate to a common value when we use a unifying theory known as supersymmetry. Supersymmetry requires that for every known particle there exists a super partner with different intrinsic spin and higher mass. A principal goal of the High Energy Physics Program is to search for such partners, especially at the Large Hadron Collider (LHC). Supersymmetry also offers the hope of unifying gravity with the other three fundamental forces of nature. This ultimate goal, to develop and confirm the theory that unifies all four forces of nature, is the underlying grand science quest motivating much if not all of the research into elementary particles and their interactions.

Other important questions remain to be answered. Why are there six types of quarks? Does the difference in the behavior of matter and antimatter predicted by the theory actually describe the world? Why is the top quark more than ten thousand times heavier than the light quarks found in the proton and neutron? Finally, what contribution can string theory make to interpreting particle behavior and bringing alternative perspectives to the Standard Model? In all of this research, advanced computational and technology research plays a vital role in experimental and theoretical efforts and future activities will be increasingly demanding of computational ability.

Research Activities

Research activities include experiments designed to explore and understand the nature and origin of the differences in behavior between matter and anti-matter, e.g., violation of symmetry in charge conjugation parity (CP) that is inconsistent with the Standard Model; experiments to determine whether neutrinos have mass and to determine their nature; search for the Higgs Boson particle predicted by the Standard Model which, if found, could help to confirm the existence of supersymmetry and possibly double the elementary particle spectrum; search for other rare particles in collisions of protons and antiprotons, protons and protons, or of electrons and protons, that reveal symmetries at ever smaller distances, supporting the theory of supersymmetry; experiments into electroweak interactions to further understand and refine the Standard Model; precision experiments designed to understand the spectrum of hadron masses and properties and supporting quark structures; research exploring how the spin structure of nucleons is affected by the spin of its internal constituents, quarks and gluons; theoretical research employing advanced computation and simulation as a framework for understanding phenomena involving fundamental particles, the Standard Model, and unification of forces; research into more sensitive, accurate, and radiation hardened particle detectors and electronics leading to technologies with spinoff applications; research into conventional and advanced particle accelerator concepts that break the constraints of current limits posed by present physical structures and materials—superconductivity, very high powered radio frequency sources, and so forth.

Accomplishments

- Researchers developed Quantum Chromodynamics and the Standard Model, which form the basis of all modern theories of the fundamental constituents of matter and the forces that bind them into the materials of the world around us.

- A Nobel Prize was awarded to James Cronin and Val Fitch for initial observation of CP violation, the asymmetry between matter and anti-matter, which is essential for the evolution of a matter-dominated universe.

- Experiments have ruled out a Higgs Boson and similar particles below 100 GeV in mass, thus helping to eliminate a significant range of theories of grand unification.

- The top quark was discovered. The top quark is the final member of the third family of elementary particles. Its high mass, almost 200 times that of the proton, is a major theoretical puzzle.

- A Nobel Prize was awarded to Martin Perl for the discovery of the tau lepton, the first indication that there are more than two families of elementary particles.

- Highly precise measurements for electroweak interactions and precision measurements of W and Z bosons' masses gave the first indications that the top quark would be very much heavier than other quarks. They also indicated a range for the Higgs Boson mass.

- The properties of hundreds of hadrons have been characterized by their mass, their intrinsic spin (or angular momentum, like a spinning top), and discrete quantum mechanical properties called parity (P) and charge conjugation parity (CP). The regularities of hadrons provided the first clues for the existence of the u, d, and s quarks.

- A Nobel Prize was awarded to Burton Richter and Samuel Ting for the discovery of the charm quark.

- A Nobel Prize was awarded to Jerome Friedman, Henry W. Kendall, and Richard Taylor for the discovery of quark substructures in the neutron and proton through deep inelastic electron scattering.

- A Nobel Prize was awarded to Leon Lederman, Melving Schwartz, and Jack Steinberger for the discovery of the existence of two distinct neutrino types. This was a critical discovery in the determination of families and led to the formation of the Standard Model.

- The discovery of bottom quark-antiquark states, and baryons containing charmed and bottom quarks established the reality of the third family of quarks and provided a lower bound on the mass of the top quark.

- Researchers discovered that most of the spin of the proton and neutron is not found in the three main quarks that make up the nucleon. The three quarks contribute about one half

of the total spin of neutrons and protons; the remainder must come from other mechanisms that are not yet completely understood.

- Precision kaon decay experiments conducted by a team of university and laboratory scientists at Fermilab led to a better understanding of CP violation, including confirmation of the existence of direct CP violation.

- An international team of university and laboratory scientists who built and utilized the CDF detector at Fermilab demonstrated the capability to perform B meson experiments in a hadron collider. The experiment made the first observation of the exotic B meson that contains a charmed quark and made a measurement that for the first time indicated that CP violation may occur in B meson decays.

- Precision measurements, by university and laboratory scientists working at Fermilab, of the W mass from the CDF and D-Zero experiments and the weak mixing angle from a neutrino experiment provided strong evidence for the validity of the Standard Model.

- Researchers developed super-string theory, including gravity, which had been a major goal of high-energy theory—the development of a "Theory of Everything."

- The modern million-turn simulation of storage rings for new machines is a significant computational tool for the design of future accelerator facilities.

- Laser wakefield and laser beat wave plasma accelerator concepts have been invented; these could be the key to future accelerators of much higher energies than existing machines.

- Proof-of-principle demonstration was accomplished for the Inverse Free Electron Laser that, by providing unique high precision sources of photons, will bring the benefits of high energy physics technology to other fields of science.

- The development of Lattice Gauge theories allowed the calculation of fundamental physics parameters from first principles. For example, estimates of direct CP violation mentioned above have been achieved.

- The invention of the strong focusing principle made the construction of high energy accelerators possible.

Nuclear Matter and Interactions

Description, Objectives, and Research Performers

Nuclear science has as its objective the understanding of nucleons and nuclei, which are the hearts of atoms and the place where almost all of the mass of ordinary matter resides. Despite the ubiquity of nuclear matter in the universe, understanding its behavior remains a major

challenge. Nuclei are assembled in stars from individual protons and neutrons, and nuclear properties are governed by their motions and interactions within the nucleus. But, at a deeper level, protons and neutrons themselves are found to have a complex structure, being composed of quarks and gluons that seem forever trapped inside. And yet, we believe quarks and gluons roamed independently during the first microsecond of the universe's existence. Quantum Chromodynamics (QCD) is considered to be an exact description of the interaction of the quarks, but the complexities of the theory make the way in which nuclear matter is constructed from quarks still mysterious. Solving this problem is essential to understanding matter under both normal and far-from-normal conditions. Extreme conditions existed in the early universe, exist in the cores of stars, and can be created in the laboratory during collisions between nuclei.

Research into nuclear matter and interactions is accomplished by a partnership of researchers from DOE's national laboratories and the nation's universities. This research is conducted primarily using heavy-ion, protin, and electron accelerators designed/tailored for these applications, funded by the Department, employing highly specialized detectors and ultra-precision electronics.

Research Challenges and Opportunities

Research in nuclear matter and interactions is mainly directed toward the challenges of understanding the strong force binding nuclei together as well as the smaller constituent particles that form the nucleons that make up the nucleus. Nuclear matter is studied under extreme conditions of temperature and pressure that may give rise to possible quark-gluon plasmas or other new states of matter. Nuclei formed at the limits of angular momentum and neutron/proton ratio probe the limits of nuclear binding. Electron scattering and electromagnetic excitation can probe details of nuclear structure and the nucleons themselves. In pursuing these research directions information can be obtained that is critical to our understanding of cosmic events such as nucleosynthesis in the Big Bang and in supernova, as well as to refine the Standard Model. Advanced computational and technology research plays a vital role in experimentation and theoretical efforts and future activities will be increasingly demanding of computational ability.

Research Activities

Progress requires a broad range of instruments and accelerators from low-energy heavy ion accelerators with stable and sometimes radioactive beams for the study of normal nuclear matter to the new Relativistic Heavy Ion Collider (RHIC) for the study of nuclear matter at super high temperature and density conditions that may be similar to those of the very early universe. Electron accelerators are essential for probing the detailed structure of small nuclear systems and within the nucleons themselves. Large underground experiments are used to measure neutrino interactions with matter. Theoretical nuclear physics research and the resulting phenomenological models are required to interpret experimental results and explain the structure, forces, and interactions of atomic nuclei.

Accomplishments

- Using the Berkeley Gas-Filled Spectrometer at the LBNL 88" Cyclotron, researchers have discovered two new elements with charge (Z) of 116 and 118, which are the

heaviest yet created. Their exceptional stability verify predictions of a new region of "superheavy" nuclei whose existence is possible by exceptionally strong shell stabilization for both the neutron and proton distributions.

- Using the Liquid Scintillation Neutrino Detector, scientists have found evidence for the existence of neutrino oscillations. Such oscillations can only occur if the neutrinos have mass. Thus, confirmation of this evidence will require significant modifications of the so-called Standard Model.

- Reactions induced by proton and heavy ions have identified a low density phase transition in nuclei, similar to the transition between liquid and gas phases in condensed matter physics.

- Established in this decade, the National Institute for Nuclear Theory at the University of Washington has become the premier international center for the development of new initiatives and collaborations in nuclear theory research.

- From early experiments that used the new Gammasphere detector, scientists have found a new and unexpected mode of collective nuclear motion, a so-called magnetic rotation, involving only a few nucleons on the surface of the nucleus.

- Recent precision measurements performed with polarized electron beams at MIT/Bates and CEBAF provide important new insight into the role of the strange quark in determining the fundamental properties of the nucleon.

- An international collaboration (HERMES), involving several U.S. Nuclear Physics groups, have presented recent results indicating that gluons are responsible for a significant fraction of the observed spin of the nucleon, based on measurements performed at the DESY accelerator in Germany.

Atoms and Molecules

Description, Objectives, and Research Performers

One of the greatest scientific accomplishments in the early twentieth century was the proof that the world around us is composed of atoms and molecules. On the scale of atoms and molecules, it is important to understand the physical properties that define their individual behavior, collective behavior, response to various external forces, and to enhance the ability to modify and alter their forms and properties for new applications. In particular, the electronic structure of materials has major consequences for the bulk properties of the materials. Two major questions pertain to the understanding of high-temperature superconductivity and giant magnetoresistance.

Theoretical and computer applications of quantum mechanics can be used to analyze the structure of materials. Tools include unique instruments such as 100 tesla, pulsed magnetic fields.

Electrons and photons are the basic probes, and the detailed knowledge thus acquired, especially in its impressive degree of precision, has wide applications in many fields of science. Magnetic optical traps have been used to create a new form of matter, the Bose-Einstein Condensate, predicted many years ago independently by Einstein and Bose on the basis of quantum mechanics. Lasers, the existence of which depends on the detailed properties of atomic systems, play an important role in this field. Research is conducted predominantly by researchers at the national laboratories and, to a lesser extent, at universities.

Research Challenges and Opportunities

Understanding the properties of solids, liquids, glasses, surfaces, thin films, and artificially structured and multicomponent materials at the atomic and molecular levels can significantly improve our ability to control and harness matter and to envision and create new materials for different applications. Challenges exist in condensed matter physics, condensed matter theory, the behavior behind particle-solid interactions, and atomic, molecular and optical science. Breakthoughs in understanding can lead to better superconductors, better semiconductors and photovoltaics, improved lasers, stronger magnets, and other material breakthroughs. Particular challenges and opportunities exist in high temperature superconductivity, including the electronic structure and properties of complex, multicomponent materials, and improved understanding of the phenomenon of giant or colossal magnetoresistance.

Research Activities

Key activities include experiments in condensed matter physics addressing magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids; experiments with optical and laser spectroscopy, photoemission spectroscopy, electrical and thermal transport, thermodynamic and phase transition, nuclear magnetic resonance, and scanning-tunneling and atomic-force miscroscopies; studies of the fabrication of structures using x-rays, design and operation of new and unique research instruments, such as the 100 Tesla Pulsed Field Magnet and the actinide photoelectron spectrometer at Los Alamos National Laboratory. New electron miscroscopy techniques are also in progress, such as development of the Z-contrast electron microscope; theory development and experiments to understand the interactions among atoms, molecules, ions, electrons, photons, and electromagnetic fields, building on capabilities at the synchrotron radiation light sources, the electron beam microcharacterization centers and the neutron scattering facilities.

Accomplishments

- A Nobel Prize in Physics was awarded to an SC-sponsored researcher for control of the motion of atoms with lasers, leading scientists to restrict the motion of atoms to that equivalent to a temperature close to absolute zero, producing an atomic cloud known as a Bose-Einstein Condensate.

- Scientists developed a new state of matter called vortex matter using a high temperature superconductor.

- Photovoltaic efficiency of solar cells was improved from 10-20% to 30% efficiencies.

- A new refrigeration/engine concept based on thermoacoustics was developed.

- Pencil-shaped organic molecules called “rodcoils” were developed with half the molecule flexible, and the other half rigid. The films that can be made with rod-coils have one sticky and one slippery surface. Such films have many potential applications, such as an anti-ice coating on an airplane wing or a blood-clot lining for artificial blood vessels.

- The recent discovery of a new polymer has renewed the possibilities for an effective membrane separation of oxygen and nitrogen (O_2 and N_2). The new strategy involves selectively stopping rotational motions of the slightly longer N_2 molecule, while allowing O_2 to continue rotating during its passage through the membrane. The polymeric membrane gives O_2 a greater diffusion coefficient compared to N_2 and allows high efficiency separation. This major advance in polymer science could enable inexpensive membrane separation technologies with broader applicability.

- Melting has been experimentally observed in an exotic material created from the magnetic vortices in supercomputers. Vortices are the small regions where magnetic fields first penetrate the superconductor, destroying the superconductivity at the vortices. Recent measurements found that these highly structured vortices behave much like particles and closely mimic matter-like states. For example, they exhibit two classic signatures of melting: a jump in density and the latent (transition) heat. Such measurements are being used to create known experimental cases to test theoretical models of superconductivity.

- Only a relatively small fraction of the huge number of possibilities for combining elements in the periodic table is used in real materials. A new strategy using fast computers and concepts from quantum mechanics has been developed to search for “winning combinations” of atoms that produce novel, stable crystal structures with improved, physical properties. This approach—Linear Expansion in Geometric Objects (LEGO)—recognizes that even complex crystal structures can be viewed as a collection of simple geometric objects such as dumbbells and triangles of atoms. The LEGO approach has predicted several unsuspected intermetallic compounds missed through conventional approaches.

- Researchers achieved first principles quantum simulations of atomic structure, electronic conductance and dynamical fluctuations in metalic nanowires, and carbon nanotubes.

- Scientists predicted novel ordered intermetallic compounds and their properties.

- A new generation of x-ray optics was developed.

Biomolecular Building Blocks

Description, Objectives, and Research Performers

At the next larger stage of matter are proteins and DNA molecules that are and contain the information for the building blocks of life. Understanding proteins and other biomolecular

building blocks is fundamental to scientific understanding of the human genome, and the genomes of plants and microbes. Understanding genomic structures has broad applications in energy, the environment, medicine, agriculture, and industry.

The ability to understand, predict, and even modify protein structure will be a central thrust of research in biology and medicine for much of the next century. New enzymes will command considerable attention as well for their medical, energy, and industrial potential. DOE has committed to sequencing a substantial fraction of the human genome as part of its contribution to the U.S. and international human genome projects. The information derived from this effort provides fundamental information and technology resources for scientists, biotechnology and pharmaceutical companies, and clinicians. Across these various areas, research is conducted at the national laboratories and at the nation's universities.

Research Challenges and Opportunities

Progress in the biomedical sciences and in biotechnology is increasingly dependent upon understanding the relationship between the structure and function of biological molecules, the dynamic and interactive behavior of biological molecules in cells, and the complete workings of a cell. This requires coordinated research at the interface of high throughput genomic DNA sequencing, biochemistry and physiology, protein structure determination, computational biology to identify genes and interpret their function and instrumentation research.

Genomic-level determinations of protein structure, function, and interaction as a follow-on to genomic DNA sequencing, will be one of the most important challenges for biologists in the coming decades, and high-speed research strategies will be required to keep pace with development and information needs on all fronts. And the schedule for decoding the human genome has been accelerated with completion of a draft sequence planned for 2000 and of the complete, highly accurate sequence planned for 2003. Ethical, legal, and social challenges resulting from the availability and use of increasing volumes of genetic information will require increased attention. Ever-faster sequencing devices and techniques will be required over time, pressing the limits of technology, computational abilities, and the underlying science that makes this possible.

Research Activities

Research activities in biomolecular building blocks are centered on the function and dynamic behavior of protein complexes since proteins generally do not work alone. Emphasis is placed on proteins that recognize and repair damage to DNA and that are involved in the bioremediation of metals and radionuclides. Research is also underway to develop a comprehensive understanding of the complete workings of a microbial cell, from the DNA sequence, to the identification of all the genes, to the production of all the proteins whose assembly instructions are contained in the genes, to the complex interaction of the genes and proteins in a cell that give the microbe its life and its unique characteristics and behaviors.

Accomplishments

- Research has led to charge-coupled device detectors (CCDs) for structural biology that have become the standard detectors for protein crystallography.
- DOE scientists were the first to reliably achieve sub-Angstrom resolution of protein structures.
- Records are being set for speed and resolution of protein structure determination at the new beamlines of the Advanced Photon Source and Advanced Light Source.
- The Joint Genome Institute, a virtual human genome center, contributed approximately 16% of the first billion units of human DNA sequence that were determined and deposited in public databases, including working draft sequences for three entire human chromosomes, 5, 16, and 19.

Portfolio Summary

This portfolio area, Components of Matter, encompasses research and supporting activities from many programs. Because of the nature of basic research, these programs and activities often crosscut many of the topics discussed above, within Components of Matter, and in many cases, they crosscut other science portfolio areas as well. The table below summarizes those core research activities that strongly support or moderately support elementary components of matter, including particles and their interactions, nuclear matter and interactions, atoms and molecules, and biomolecular building blocks. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities
Adv. Particle Accelerator Concepts
Advanced Computing and Communications Facility Operations
Advanced Computing Software and Collaboratory Tools
Applied Mathematics
Atomic, Molecular, and Optical Science
Computer Science to Enable Scientific Computing
CP Violation - B-Meson System
CP Violation - K-Meson System
Electroweak Interactions
Experimental Condensed Matter Physics
Facility Operations: AGS
Facility Operations: Fermilab
Facility Operations: SLAC
General Technology: Accelerator R&D
General Technology: Detector R&D
Hadron Spectroscopy

Heavy Ion Facility Ops. & Constr.
High Energy Physics Theory
High Performance Computer Networks
High Throughput DNA Sequencing
Low Energy Facility Ops. & Constr.
Medium Energy Facility Ops. & Constr.
Microbial Genomics
Neutrino Mass and Mixing
Nuclear Structure & Astrophysics - Low Energy Nuclear Physics
Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics
Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics
Resources and Tools for DNA Sequencing and Sequence Analysis
Scientific Computing Application Testbeds
Search for Higgs & Supersymmetry
Spin Structure of Nucleons
Strong Interactions, Supersymmetry & Particles
Theoretical Nuclear Physics
Theory & Simulations of Matter, Engineering Physics
Understanding and Predicting Protein Structure

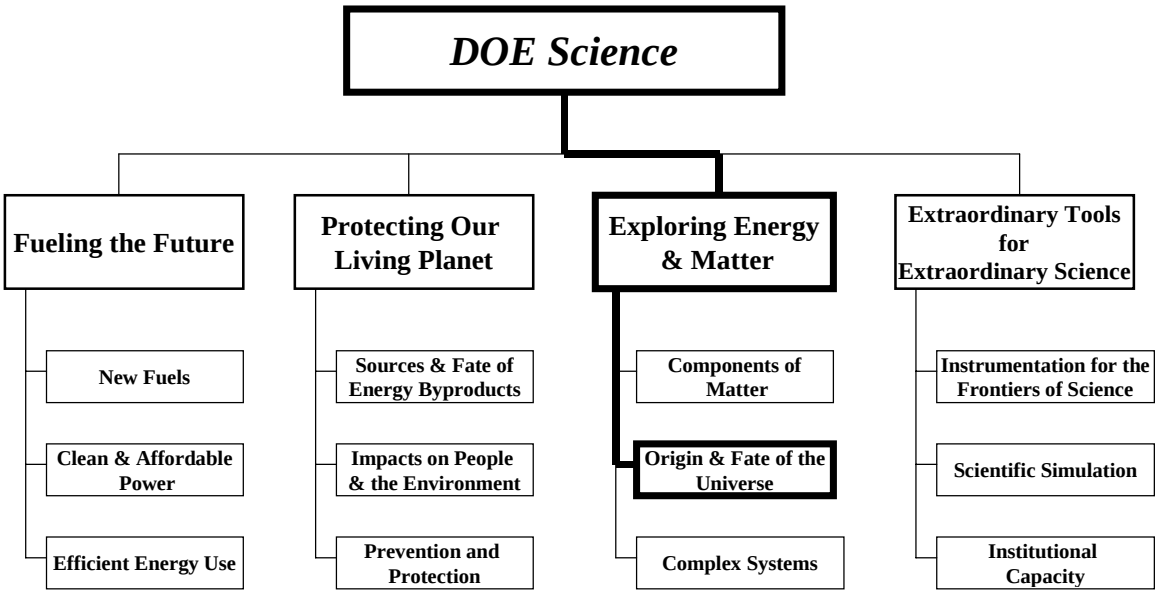
Moderately Supportive Core Research Activities
Advanced Fusion Materials Research
Analytical Chemistry Instrumentation
Environmental and Molecular Sciences Laboratory (EMSL)
General Plasma Science
General Purpose Plant & Equipment (GPP/GPE)
Heavy Element Chemistry
Materials Chemistry
Multiprogram Energy Lab Facilities Support (MELFS)
Natural and Accelerated Bioremediation research Program
Neutron and Light Sources Facilities
Neutron and X-Ray Scattering
Oak Ridge Landlord
Particle Astrophysics & Cosmology
Photochemistry and Radiation Research
Production DNA Sequencing Facility
Science Education Support
Small Business Technology Transfer (STTR) Program
Structural Biology Research Facilities
Structure of Materials
Understanding Gene Function

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 9

Origin and Fate of the Universe

Scientific Challenge: ***To understand the evolution of the universe from fundamental laws.***



Chapter 9
Origin and Fate of the Universe

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Understanding the origin and fate of the universe seeks to answer the eternal questions: Where did we come from? Where are we going? What is the ultimate fate of the universe? The expansion of the universe, originally observed by Edwin Hubble in the 1920s, and the Cosmic Microwave Background Radiation (CMBR), discovered by Penzias and Wilson in 1962, gave rise to the Big Bang Cosmology, which theorizes that the universe began with an enormous concentration of radiant energy in an extremely small volume at an extremely high temperature (a singularity), which then expanded and cooled. After an inflationary era in which the expansion was very rapid, the expansion settled down to the steady rate observed by Hubble; the radiant energy condensed to form matter as it cooled, leaving behind the 2.7 degree CMBR that we observe today. Neutrinos also cooled to form a similar background, which has yet to be detected.

The original discovery by Hubble indicated that the velocity of recession of distant galaxies is proportional to the distance from Earth. It is as though we are on the surface of a large balloon, which is expanding at a constant rate. Very recently, observations of distant supernova suggest that there is an additional term in the expansion rate originating from a cosmological constant ("dark energy"), which can be effectively regarded as a universal repulsive force.

Modern theories of the basic building blocks of matter and the fundamental forces between them tell us a great deal about the stages of matter formation. In the earliest few seconds, the cooling radiation, consisting of photons and gluons, condenses to form pairs of fundamental particles, quarks and leptons, and their corresponding anti-particles. This is the so-called quark-gluon plasma, which the RHIC facility hopes to detect in collisions of heavy nuclei with one another. At a later stage, quarks and gluons condense to form nuclei, which then form galaxies and stars; our knowledge of high energy and nuclear physics enables us to gain insight into these processes. One in particular, the evolution of a world dominated by matter, rather than an equal mixture of matter and anti-matter, as it must have been in the beginning, is intimately related to the issues to be studied in DOE-sponsored research. Another, the question of whether the Universe will continue expanding or will slow down and start to contract, is closely related to the problem of Dark Matter and its connection with new families of particles.

In the beginning of the Big Bang, pure energy was confined to a tiny space. And the energy expanded and cooled and condensed into matter, so that it was a thick soup of photons, leptons, quarks, their anti-particles, and gluons forming a plasma. Then space inflated rapidly and, because the laws of physics did not respect the symmetry between particles and anti-particles in a mirror, photons, leptons, quarks began to predominate over anti-particles, and the universe became a universe of matter. Then it expanded more slowly, and the quarks condensed to form protons and the protons to form light nuclei in a sea of photons.

As the sea of photons cooled, it became a universal background, detectable today as the Cosmic Microwave Background, first detected by Penzias and Wilson in 1962. Photons do, however play an important role in the synthesis of light nuclei, such as helium and lithium, from primordial hydrogen. Because of tiny directional asymmetries in the photon and lepton background that arose in the inflationary era, matter began to cluster into clouds of hydrogen gas under the influence of mutual gravitational attraction. Further expansion and cooling led to separation of the gas into galaxies and stars.

The actual process of galaxy formation is a problem ideally suited to computational physics. The basic law of gravitational attraction is well understood and so can be applied to the large-scale situation in which vast numbers of particles, predominantly hydrogen atoms, interact with one another and clump together. This clumping is thought to reflect the universe's small matter asymmetries, asymmetries that have indeed been observed by the COBE satellite, and amplifies them to form the galaxies. From observing rotation curves, scientists know the universe contains a great deal of dark matter, which does not shine like the stars, but which makes its presence known through its gravitational interactions. The nature of this matter—brown dwarfs, unknown elementary particles, or massive neutrinos—is not known, and its role in galaxy formation is not fully understood. This dark matter problem is one of the principal problems of astrophysics and particle physics.

Within the stars, gravity produced further condensation which caused the temperatures in the stars to rise until they were hot enough to make the hydrogen fuse to form heavier elements. Because of the Curve of Binding Energy—a major property of the strong nuclear force—the fusion process in stars went all the way to iron and then stopped.

Stars with heavy iron cores tend to collapse under their own weight and explode, blowing off their excess material in a gigantic supernova explosion and leaving behind a dense neutron star or black hole. The explosion of some supernovae becomes visible to the naked eye over a short period of time, but neutrinos carry off most of the gravitational energy released in these explosions. Such neutrinos were detected in 1987 by large water Cerenkov detectors originally built to search for proton decay. Stellar fusion and explosions are responsible for the production and distribution of elements heavier than helium and lithium throughout the universe.

The precise mechanism of supernova explosions has been a subject of investigation for many years and is still not completely understood. While neutrinos are important, it is not entirely understood how they help to blow off the outer layers of the exploding star. Understanding this phenomenon represents a major computational challenge.

Elements heavier than iron are much harder to produce in stellar processes and are therefore relatively rare. Generally speaking they are made by neutron capture processes on iron and heavier elements, followed by beta-minus decay, which turns a neutron into a proton and thereby changes the chemical properties of the final nucleus. Some neutron capture processes (r-processes) proceed rapidly, and others (s-processes) tend to be slow. Scientists can learn a great deal about these naturally occurring processes by bombarding the parent nuclei in the laboratory with neutrons and with heavier, radioactive species.

The cosmic dust blown off by supernovae begins to accumulate in gravitationally bound orbits around stars and will, from time to time, coalesce into planets like those of the Earth's solar system. Planetary structures are too small to generate nuclear reactions, as stars do, so they can remain stable and absorb energy from the radiation emitted by the star. Under the right conditions, a planet may acquire an atmosphere of light gaseous elements, like that of the Earth, which shields it from the most harmful effects of stellar radiation, and even traps energy carried by it.

As the starlight is absorbed it can, through the process of photosynthesis, lead to the creation of biological molecules combining carbon and hydrogen and rarer elements. Much remains to be learned through laboratory experimentation regarding the formation and evolution of life on the Earth, and about the possibility of life in other planetary systems.

Beginning of the Cosmos

Description, Objectives, and Research Performers

During recent years, a close connection has developed among the research areas of high energy and nuclear physics, cosmology, astrophysics and gravity. Pertinent interdisciplinary questions concern the early moments of the Big Bang expansion of the universe as it flowered into existence, the microscopic origin of the observed cosmic asymmetry between matter and antimatter, the nature of dark matter which is thought to dominate the matter content of the universe, the possibility of "dark energy", the formation of structure in the universe, and the ultimate fate of the Universe (whether it will expand indefinitely, and at what rate, or ultimately contract, and whether there might be multiple universes). This research is carried out at universities and national laboratories.

Research Challenges and Opportunities

A major goal is to determine the fundamental parameters of the universe itself, in the context of Einstein's Theory of General Relativity. During the past few years there has been substantial theoretical progress in constructing candidate theories of quantum gravity (so-called super-string theories). These promise deeper understanding of black holes and even of the Big Bang itself. Many important questions remain unanswered. How did the universe evolve in its earliest moments of existence? Does the universe have curvature? Is there a cosmological constant ("dark energy")? Recent experiments on Supernova redshifts, utilizing techniques from High Energy Physics, seem to have some indications for "dark energy." This has led to reformulations of the early universe scenarios. Other challenges include understanding the origin of the observed baryon asymmetry in the universe (matter over anti-matter), and the origins of galaxies.

The search for dark matter provides a clear example of the deep connections between High Energy Physics and cosmology. The inflationary theory of the early universe together with astronomical measurements, favor a total density of the universe that is nearly critical. Observations tell us that most of the critical density cannot be luminous matter. Direct observation of galactic rotations indicate significant amounts, perhaps half of the galactic mass, consists of non-luminous matter. Collectively, this is called dark matter. Candidates for dark matter include massive neutrinos, and/or stable relics of the Big Bang. Such relics are predicted in theories of CP violation, supersymmetric theories and strong-interaction theories. The discovery of any one of these particles would indicate physics beyond the Standard Model, and would represent a significant advance in understanding the origin and evolution of the universe.

Research Activities

Experiments search for particle dark matter, survey large redshift supernovas and galaxies, seek to understand the small anisotropy of the cosmic microwave background, study the highest-energy cosmic rays, and search for proton decay, magnetic monopoles and neutrino masses. These experiments are conducted mostly far away from accelerators—at remote sites on mountain tops, deep mines, deep ice, high plains, or in space.

Accomplishments

- Scientists have established connections that show how the early universe evolved from a dense plasma of quarks and gluons to the vast regions of empty space in the universe. The relative amounts of hydrogen, helium and other light elements can be calculated on the basis of known nuclear properties together with observed properties of neutrinos.

- Scientists have measured in deep underground laboratories neutrinos produced by cosmic rays bombarding the atmosphere and have deduced that neutrinos may have mass. More direct accelerator-based measurements are being mounted to verify this major discovery. This was rated one of the two top discoveries of 1998 by *Science* magazine.

- Researchers formulated the theory of inflation, according to which the universe in its earliest moments went through a period of rapid expansion, enabling quarks and gluons to condense into neutrons and protons, forming the basis of atomic matter.

- Val Fitch and James Cronin were awarded the Nobel Prize for the discovery of CP violation, or the lack of symmetry between particles and anti-particles. This lack of symmetry leads to a present-day universe which is dominated by matter, rather than one equally populated by matter and anti-matter.

- High energy physics techniques for detecting photons have been used by astronomers and astrophysicists at Lawrence Berkeley National Laboratory to perform a survey of distant supernovae, one as far as ten billion light years away, to determine their distance and speed of recession from Earth. The further away the supernovae are, the longer it takes the light to reach the earth; thus the distant supernovae enable us to look at the universe at an earlier time, billions of years before the present era. The startling result of this research, confirmed by an independent survey in Australia, is that the universe appears to be expanding at an increasing rate as time goes by, that it will go on expanding forever, and that there is a “dark energy” component of the universe. This research has just been rated the top discovery of 1998 by *Science* magazine.

- According to modern theories of particle physics, the evolution of a matter-dominated universe from the Big Bang requires that the proton not be an absolutely stable particle, but must be able to eventually decay into lighter particles after a very, very long time. Present day experiments are searching directly for proton decay, but have failed to detect it thus far, indicating that a proton must live more than one hundred thousand billion billion billion years!

- The techniques of nuclear physics and high energy physics are being used today to search for other relics of the Big Bang, including relic neutrinos, magnetic monopoles, and other particles. Some of these may be related to the problem of dark matter, matter that we detect by its gravitational properties, but does not emit light or any other electromagnetic radiation

- The observational and computational techniques of high energy and nuclear physics have been used by the Sloan Digital Sky Survey to observe the most distant quasar, several billion light years away.

Creation of Nuclei and Matter

Description, Objectives, and Research Performers

Understanding the evolution of the universe beyond the first moment of the Big Bang is a matter of reconstructing events on the basis of the known laws of physics. After the initial singularity, a sequence of events had to take place as the universe cooled, in order that the universe came to be as it is today. Exactly what happened is the subject of intense theoretical speculation. In particular, scientists theorize that, very quickly after the Big Bang, the hot, dense matter (of quarks, antiquarks, leptons, antileptons, and other particles) created in the initial disturbance of the vacuum underwent a phase transition to normal matter, the stuff that makes up today's universe. In the sequence of events almost all of the antimatter was annihilated, leaving only a small excess of matter. This process requires CP violation, observed in high energy physics experiments, violation of baryon number, e.g., proton decay (not observed as yet), and/or lepton number (also not observed), and thermodynamic non-equilibrium. Protons and electrons are among the most abundant particles in the universe, numbering approximately 10^{80}. They are also extremely stable and may not decay.

Neutrinos left over from the initial annihilation are also in principle detectable, but in practice they have eluded detection. The light atoms left over represent all of the normal matter in the universe, and some of these gradually coalesced into galaxies even as the universe was expanding. The relative abundance of the light atoms is determined by the interaction dynamics. For example, the synthesis of nuclei in the early cosmos and the relative abundance of the elements D, ^{4}He, and ^{7}Li depend on the number of species of light neutrinos, and astronomical observations limits their number to be about 3. This is exactly the number observed in high energy physics experiments, and exactly the number of neutrino species in the Standard Model. This research is carried out at universities and national laboratories.

Research Challenges and Opportunities

The challenge is to find and measure the relevant entities that shed light on the early creation of matter in the universe. This includes recreating and studying in the laboratory the behavior of nuclear matter at temperatures and densities comparable to those that existed after the Big Bang. Understanding the origins of CP violation and baryon asymmetry is central to this activity. Understanding the relative abundance of the light atoms is also very important. For example, almost all the hydrogen and deuterium in the universe today was produced in the Big Bang.

Research Activities

Using relativistic heavy ion collisions, nuclear physics experiments study the behavior of hot, dense nuclear matter and search for evidence of a "quark-gluon plasma" and the phase transition to normal hadronic matter. High energy physics experiments have measured the proton lifetime to be more than 10^{32} years, for the most probable modes of decay. Theories that unify the electroweak and strong forces predict that protons decay with a lifetime in a range perhaps just beyond the reach of current experiments. Along with proton decay, these theories predict the possible existence of magnetic monopoles, relic particles created in the Big Bang carrying units of magnetic charge, analogous to electric charge. Magnetic monopoles have been sought in high energy physics experiments, so far without success. Finally, these theories predict the possible existence of even stranger objects, among them cosmic strings, of enormous length and mass. These may have existed since the Big Bang, and if so would have been instrumental in the formation of galaxies. Other experiments in high energy and nuclear physics have searched for violation of lepton number, and have set stringent limits on such processes. Other experiments are proposed to search for antimatter in cosmic radiation.

Accomplishment

- Knowledge of nuclear physics and high energy physics has enabled scientists to explain the abundances of light elements in the early universe, and to calculate the ratio of the number of hydrogen atoms to the number of photons in the universe, roughly one to one billion. These ratios are influenced by the number of different kinds of neutrino and indicate that no more than three different kinds exist. This result is consistent with the direct measurement of the number of neutrino types made by studying the Z bosons at the LEP electron-positron collider at CERN.

- Experiments have established the properties of dense "normal" nuclear matter at temperatures below that expected for the production of a "quark-gluon plasma." This knowledge is essential for the discovery and observation of the quark-gluon plasma state of nuclear matter at higher energies and temperature at the RHIC facility.

- Radioactive beams of ^{18}F have been produced at the ATLAS facility at ANL to measure proton capture and reaction cross sections, which provide very stringent constraints to nuclear astrophysicists trying to understand the production of nuclei heavier than oxygen.

- Developing methods necessary to perform experiments at energies that correspond to the conditions in the core of a star, neutron capture in ^{7}Li has been carefully measured at the Oak Ridge Electron Accelerator (ORELA). The results of this important experiment resolved a significant discrepancy in the data needed for the understanding of the formation of heavy elements like carbon, nitrogen, and oxygen in the evolution of the universe.

Evolution of Astrophysical Structures

Description, Objectives, and Research Performers

Even as the universe expanded from its first moments, the radiation remaining from the matter-antimatter annihilation was not completely uniform and isotropic. Tiny anisotropies in those moments, a few parts per million, are evident today in observations of the anisotropy of the microwave background. These tiny imperfections could have become the seeds of galaxies according to current theories. Further, neutrinos, being part of this radiation, could also participate in the seeding, particularly if they themselves carry mass. High energy and nuclear physics experiments are currently showing some indications that neutrinos might carry a tiny mass. These anomalous regions of higher radiation density created gravitational potential wells that gradually attracted matter, which in turn caused a gravitational attraction for more matter.

As the clouds of light atoms flowed into galactic and super-galactic clusters of matter, some regions of self-gravitating matter coalesced and heated up through mutual interactions, and the first stars were born. This process was repeated hundreds of millions of times in each galaxy, for billions of galaxies. Understanding this process is a major objective of astrophysics, and understanding the underlying seeding from the early cosmos is a central goal of cosmology.

The evolution of stars and galaxies is the focus of astrophysics, aided by astronomical observations. The life cycle of a star is a fascinating subject in itself. In falling (mostly hydrogen) gas contracts and heats up under the influence of gravity, and is ignited by nuclear interactions. Protons, the nuclei of hydrogen atoms, fuse to produce deuterium nuclei that further interact with protons to produce helium. Helium cooks in the inferno, and through interactions with other nuclei, synthesis of heavier elements up to carbon occurs. Then carbon nuclei interact with other nuclei producing even heavier elements, all of the elements in the Periodic Table. Energy is produced in many of these interactions, which heats up the star and produces light and other radiation, such as neutrinos and cosmic rays. Understanding these processes, and the critical nuclear reaction rates which drive them, is a major focus of the nuclear physics program.

The end of the life cycle of a star can be spectacular, as a dying star goes through the red giant phase, and as the nuclear fires start to burn out, contracts under gravity, and in the case of larger stars, explodes into a supernova. This process results in the core of the star contracting to nuclear densities, a neutron star or pulsar as it is known from its radio wavelength radiation. In even heavier stars, the core will contract to a black hole. The latter is a meeting place and testing ground for quantum gravity, as black holes can radiate particles through a quantum process. Thus the ultimate description of a black hole must properly combine gravity and quantum mechanics. Recent work by super-string theorists has resulted in a calculation of the entropy of a black hole from a microscopic quantum theory. There are, however, many unanswered questions about the dynamics of supernovas and black holes. Understanding the explosion of a supernova will require detailed calculations of the transport of neutrinos through dense nuclear matter. Some interesting current experiments attempt to detect high energy gamma rays, and to detect the very highest energy cosmic rays, both of which may come from astrophysical sources powered by black holes. Other experiments have detected the neutrino radiation from a nearby supernova (SN1987A). Furthermore, our present understanding of element formation has the

elements heavier than iron formed during the brief period of supernova explosions. Models for these processes requires knowledge of nuclear reaction rates at relevant stellar energies and with nuclear species far from the region of stable nuclei. Research in these areas is conducted at universities and national laboratories.

Research Challenges and Opportunities

The challenge is to understand the origin and evolution of stars and galaxies from first principles, and to understand the production rates of the elements observed in nature. Researchers seek to identify relevant experiments and theories. For example, determining whether neutrinos have mass not only relates to the understanding of the Standard Model, but also to the formation of galaxies. Likewise, dark matter may relate to extensions of the Standard Model (e.g., supersymmetry, grand unified theories, super-strings), and also to galactic rotations. The observed elemental abundances relate directly to a number of critical nuclear reaction rates.

Research Activities

Experiments and theoretical investigations that bear on the understanding of the formation and evolution of astrophysical structures are ongoing. Direct searches are underway for dark matter, neutrino mass, magnetic monopoles, supernovas, and high energy cosmic. The calculations relating to Black Holes, supernova dynamics, and the seeding of galaxies comprise much of the current theoretical activities. New accelerator facilities and instrumentation are being developed to measure critical nuclear reaction rates for element formation. In particular, the concept is being developed for a new accelerator, the Rare Isotope Accelerator, that will produce intense radioactive beams far from stability.

Accomplishments

- William Fowler was awarded the Nobel Prize for his theoretical and experimental studies of nuclear reactions of importance in the formation of the chemical elements. His work, together with experimental and theoretical efforts in recent years, has resulted in the basic framework for understanding the production of the chemical elements of the universe.

- The SuperKamiokande detector has found strong evidence for neutrino mass—a result just rated as one of the top ten scientific discoveries of 1998 by Science Magazine—and this may provide part of the missing mass, or dark matter of the universe. New experiments are being mounted at accelerators to determine the mass parameters. Also, a new detector, KamLAND, is being constructed by a Japanese-American collaboration to measure the mass parameters of reactor-generated neutrinos. The Big Bang has left behind a sea of relic photons that have been measured with great accuracy by COBE satellite. Tiny inhomogeneities, at the level of one part in ten thousand have been detected, and these appear to be responsible for the formation of the galaxies we see today.

- The Sloan Digital Sky Survey has revealed the most distant quasar ever discovered.

- Precision measurements of giant resonance excitation in nuclei using the Texas A&M Cyclotron have led to an accurate determination of the compressibility of nuclear matter at the density of ground state nuclei. This information is an important experimental ingredient in developing the equation of state of nuclear matter, which is needed in models of supernova evolution.

Formation of Life

Description, Objectives, and Research Performers

As the universe evolved, so too did life, from a collection of complex biomolecular structures to simple organisms capable of replication. With the discussion just a few years ago of possible simple life on Mars, our view of the universe, and of our own uniqueness on planet Earth, continues to change. Similarly, exploration of our own planet, aided by science and technologies developed at the Department of Energy, are radically changing our view of the formation of life and the possibilities of life in extreme environments. For example, science that began as an initial outgrowth of the atomic era—an era challenged with understanding the effects of radiation on living organisms—recently culminated in the identification of a new form of life on Earth, a third kingdom of living organisms known as Archaea (from the Greek word for ancient). Archaea are distinct from other microbes in that they lack a cell nucleus. DOE's Microbial Genome Program performed the genomic sequencing of the first Archea, *Methanococcus jannaschii*, a methane-producer that dwells in the extremely harsh conditions of "white smokers" on the sea floor. This genomic sequencing confirmed for the first time the emerging belief that the organism was part of a new, third kingdom. This information, coupled with similar information from sequencing of other organisms within Archaea, shows promise and may lead to several commercial products, such as heat-stable enzymes for the textile, paper, and chemical industries; systems that produce methane for chemical feedstock and renewable fuels; and tailor-made proteins that can be used to clean toxic contaminants from the environment.

Further research into the details of key microbes will enable insights into the workings of these minimal forms of life, some of which inhabit environments notable for extremes of temperature, pressure, acidity, and salinity, as well as high concentrations of toxic chemicals and even high fluxes of radiation. Beyond improvements in our understanding of evolution and the origins of life, benefits will undoubtedly extend to medicine, agriculture, industrial processes, and not least, environmental bioremediation—the latter an important issue at some Department of Energy facilities. Research is carried out at national laboratories and universities.

Research Challenges and Opportunities

Research on this topic reveals many challenges and opportunities, but understanding the structure, function, and regulation of genes at a genomic scale will be one of the great challenges in biology for the next several decades.

In addition, the identification and understanding of new organisms with interesting and useful properties will provide many new opportunities. Often nature is truly one of the best and most creative inventors. A particular challenge is to understand simple living organisms that are capable of seemingly incredible feats of self-preservation in the face of extremely harsh

conditions, and to synthesize and harness these processes for various applications. One such organism is *Deinococcus radiodurans*. It prospers even when exposed to doses of radiation that would kill the typical microbe many times over. The secret is not avoidance of damage, but rather a remarkably efficient DNA repair mechanism—one that might be engineered to allow bioremediation of dangerous radioactive wastes. Another challenge is to expand and convert our scientific knowledge of *Methanococcus jannaschii* into useful expressions, such as medical, industrial, and energy applications.

Overall, advances in genomics, structural biology, instrumentation and automation, as well as the use of model organisms, pose both research challenges and opportunities in science.

Research Activities

Research activities include the identification of primitive microorganisms with potentially useful properties for bioremediation, as well as industrial, medical, and agricultural applications, with particular attention devoted to simple organisms capable of surviving in extreme environments; continued examination of intracellular processes (including life cycle and repair mechanisms, and enzymes) that regulate the life control of simple organisms; potential evolutionary aspects of simple organisms; and development of methods to accelerate genetic sequencing and structural biology research leading to high throughput technologies for providing information on gene structure.

Accomplishments

- Scientists confirmed the existence of a third form of life, the Archae, a branch at the root of life on Earth, with the complete genomic sequencing of the DNA from *Methanococcus janaschii*.

- Complete genomic sequencing of *Mycoplasma genitalium*, the smallest known free-living organism—a key to understanding the minimum requirements for life.

- Complete genomic sequencing of Archae from different families on this branch of the tree of life. These include *Archaeoglobus fulgidis* (involved in oil well souring), *Methanobacterium thermoautotropicum* (another methane producer), and an Archae that can survive at extremely high temperatures, *Pyrobaculum aerophilum*.

- Complete genomic sequencing of Deinococcus radiodurans, dubbed Conan the bacterium by the media, with potential uses in the cleanup of DOE waste sites.

Portfolio Summary

This portfolio area, “Origin and Fate of the Universe,” encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activities that strongly support or moderately support Origin and Fate of the Universe, including beginning of the cosmos, creation of nuclei and matter, evolution of astrophysical structures, and formation of life. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications

for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

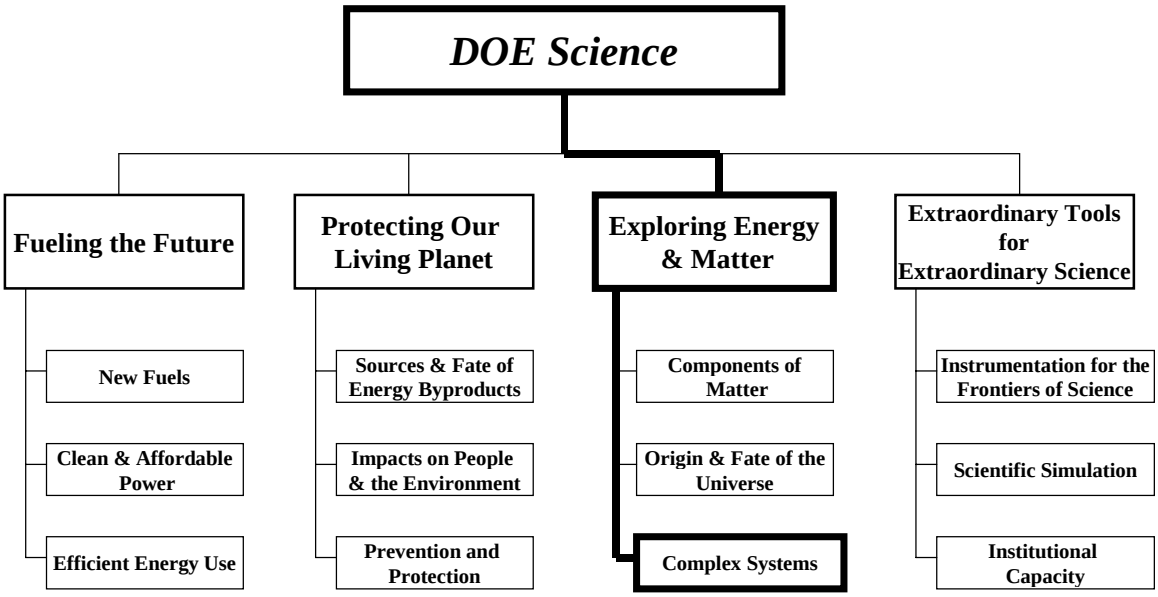
Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations
Applied Mathematics
Computer Science to Enable Scientific Computing
CP Violation - B-Meson System
CP Violation - K-Meson System
General Plasma Science
Heavy Ion Facility Ops. & Constr.
Low Energy Facility Ops. & Constr.
Microbial Genomics
Neutrino Mass and Mixing
Nuclear Structure & Astrophysics - Low Energy Nuclear Physics
Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics
Particle Astrophysics & Cosmology
Plasma Theory and Computation
Scientific Computing Application Testbeds
Theoretical Nuclear Physics

Moderately Supportive Core Research Activities
Atomic, Molecular, and Optical Science"
Electroweak Interactions
General Purpose Plant & Equipment (GPP/GPE)
Hadron Spectroscopy
High Energy Physics Theory
High Performance Computer Networks
Medium Energy Facility Ops. & Constr.
Multiprogram Energy Lab Facilities Support (MELFS)
Oak Ridge Landlord
Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics
Science Education Support
Search for Higgs & Supersymmetry
Spin Structure of Nucleons
Strong Interactions, Supersymmetry & Particles

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 10
Complex Systems

Scientific Challenge: ***To understand and control complex systems of matter, energy, and life.***



Chapter 10
Complex Systems

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Much of the research of the past 50 years has been devoted to solving very difficult problems in idealized, simple systems. The challenge now is to use that knowledge to better understand complex systems involving collective phenomena and adaptive systems.

Radically different, complex systems appear when many entities come together, interact or adapt. Complexity in natural systems typically arises from the collective effect of a very large number of components. At present, it is often impossible to predict the detailed behavior of any single system's component, or, in fact, the precise behavior of the complete system. But the system as a whole may nevertheless show definite overall behavior, and this behavior usually has several important features. A wide variety of systems exhibit overall behavior. For example, the many aspects of magnetic phenomena, ferromagnetism, anti-ferromagnetism, and spin waves are attributable to the collective behavior of many spins; and the ability to think and adapt to surroundings is the result of complex behavior of many neurons.

The time is ripe for further emphasis in understanding complex systems because of new theoretical and experimental methods and results. For example, third generation synchrotrons allow measurement of weak signals and determination of structures of complicated molecules and materials. We can now study interfacial phenomena directly using intense x-ray beams. Increases in computational power make it possible to do realistic simulations of non-ideal systems in reasonable times. New synthesis techniques, such as combinatorial chemistry, make it possible to synthesize large numbers of compounds very quickly to search for combinations with certain properties and to test and refine theory. Combined, these techniques are creating an opportunity to bridge the gap in understanding between atomic and molecular properties and the bulk structural and mechanical properties of materials. and to create new, better materials.

Whole genome sequencing and analysis are providing a new paradigm for biological research. The ability to determine the complete genetic potential of an organism permits a context for integrating individual molecular, biophysical, biochemical, cellular and physiological processes and events into a fuller understanding of living systems. The understanding of biological systems at ever-increasing levels of complexity promises to usher in a new age in biological research.

Collective Phenomena

Description, Objectives, and Research Performers

The challenge at the frontiers of basic research is to obtain fundamental understanding of increasingly complex systems. Systems composed of many elements show some unique behavior patterns, which may be called "collective phenomena." Recent progress in science sheds new light on these complex phenomena. Classical physics considers systems of particles; now, more sophisticated elements are coming within our scope of study. For example, scientists are systematically analyzing fundamental paradigms of collective phenomena; relevant research is being conducted on the physics of nonlinear waves (solitons), fluid dynamics, plasma physics, spectral theories, phase transitions, turbulence, and self-organization in complex systems. Such research involves multidisciplinary and interdisciplinary efforts and holds the promise of delivering revolutionary breakthroughs. It bridges the gap between an atomic level understanding (reductionist view) and a continuum mechanics understanding (classical view) of

complex and collective phenomena. Research is conducted predominantly at national laboratories and universities.

Research Challenges and Opportunities

Important areas of inquiry in the field of collective phenomena include the following: (1) Classes of non-equilibrium materials that will be key elements of the next generation of energy technologies pose new challenges and opportunities because of their complexity. (2) Despite their importance, catalytic processes are not sufficiently well understood to allow for the rational design of new catalysts. Models for catalytic action are limited in scope and applicability. (3) Even though photosynthesis has been studied for decades, we still do not completely understand it nor have we been able to duplicate or improve on it. This one example of the control of entropy — the ability to mimic the functions of plants — remains one of the outstanding challenges in the natural sciences. (4) A major unsolved problem is the physical mechanism that makes high-temperature superconductivity possible. (5) A challenging issue is giant or colossal magnetoresistance. (6) We understand single atoms, molecules, and pure crystals fairly well; but, when we go beyond these simple systems to larger more complex systems, our understanding is limited. Understanding phenomena over wide timescales is also important — from femtoseconds in spectroscopy, to decades in the regulatory system of plants, to thousands of years in radioactive waste disposal.

Research Activities

Office of Science-sponsored research spans the materials, chemical, plasma, geological, engineering, geological plant and microbial sciences. Research in chemistry, materials, geosciences, and biosciences covers lengths from the atomic scale to the cellular scale to the meter scale and times from femtoseconds to millennia. For example, theory and simulation of plasma behavior in both magnetic and inertial fusion is complex because of the many orders of magnitude in spatial and temporal scales involved. Examples of research into collective phenomena include non-equilibrium systems, functional synthesis, control of entropy, strongly coupled systems, and heterogeneous systems.

Non-equilibrium systems. Areas under investigation include high-temperature superconductors, which are complex compounds of four or more elements that are not stoichiometric with respect to oxygen; and the glassy metal state, which has many desirable properties, but no long range order or symmetry. Researchers are discovering that many interesting and useful properties exist in atomic and molecular arrangements that have minimal dimensions, such as those found in thin films, membranes, and quantum dots. Other examples include polymers, molecular magnets, biomolecular materials, and new inorganic materials, all of which are important in applications such as fuel cells, batteries, membranes, catalysis, electrochemistry, and photoabsorption. A very exciting area of research is in biomolecular materials. Biological models are being used to make better polymers; to develop self-assembled, three-dimensional structures; to make very sensitive sensors, and to deposit hard inorganic coatings.

Functional synthesis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered

in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes.

The control of entropy. Photochemistry research investigates, at the molecular level, fundamental processes that capture and convert solar energy. This research encompasses organic and inorganic photochemistry, electron and energy transfer in homogeneous and heterogeneous media, photocatalysis, and photoelectrochemistry. Naturally occurring photosynthetic reaction centers and antenna systems are studied as models of biomimetic/photocatalytic assemblies that can carry out efficient photoinduced charge separation.

All living systems control entropy. Basic research on plants includes photosynthetic mechanisms and bioenergetics in algae, higher plants, and photosynthetic bacteria; control mechanisms that regulate plant growth and development; fundamental aspects of gene structure, function, and expression; plant cell wall structure, function and synthesis; and mechanisms of transport across membranes. Research in these areas seeks to define and understand the biological mechanisms that effectively transduce light energy into chemical energy, to identify the biochemical pathways and genetic regulatory mechanisms that can lead the efficient biosynthesis of potential fuels and petroleum-replacing compounds, and to elucidate the capacity of plants to remediate contaminated environments by transporting and detoxifying toxic substances.

The research focus in the microbiological sciences includes the degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of microbial growth and development, thermophily, e.g., bacterial growth under high temperature, and other phenomena with the potential to impact biological energy production, conversion and conservation. Organisms and processes that offer unique possibilities for research at the interface of biology and the physical, earth and engineering sciences also need to be studied.

Strongly coupled systems. Research aimed at a fundamental understanding of the behavior of materials includes experimental measurements to determine electronic structure, transport properties, phase transitions, mechanisms for high temperature superconductivity, complexity in electronic interactions, self-organization of electronic states. The materials examined include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The measurements include optical and laser spectroscopy, photoemission spectroscopy, electrical and thermal transport, thermodynamic and phase transition measurements, nuclear magnetic resonance, and scanning-tunneling and atomic-force microscopies. The development of new techniques and instruments including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy are necessary to understand coupled systems.

Fusion involves complex coupling of particles and fields. Although there has been marked progress in understanding macroscopic equilibrium/stability and turbulence and the associated transport in plasmas, improved theories and simulations are needed to quantitatively predict the behavior of fusion plasmas. Current models of equilibrium and stability must be extended to be fully three-dimensional and to include fluid and kinetic effects. Simulations of ion turbulence and transport should be extended to include electromagnetic effects and improved models of

electron dynamics. In addition, new approaches to understanding energy transport in tokamaks, such as Self-Organized Criticality, are being investigated to understand their applications to fusion plasmas. Ultimately, integrated models, capable of complete simulation of both magnetic and inertial confinement systems, must be developed.

Heterogeneous systems. New research involving advanced computational and experimental approaches for treating complex mineral-fluid interactions will improve the understanding of fundamental processes and their interactions over a wide range of space and time scales needed for quantitative predictions of the consequences of transport and use of energy and material within the Earth's crust.

Accomplishments

- Proof of a thermodynamic first-order transition from a solid-like vortex lattice to a vortex liquid in a high temperature superconductor is leading to development of a new state of matter called vortex matter. The nature of the transition is significant for fundamental theories of phase transitions and also for practical applications of superconductivity.

- A metal-insulator transition has unexpectedly appeared in a MOSFET (Metal-oxide-semiconductor- field-effect-transistor) subject to strong electric fields at low temperatures. This is remarkable, because a MOSFET operates as an ultrathin sheet of electrons on the surface of the silicon semiconductor and, according to established theory, should not conduct at very low temperatures. This behavior is very consistent with what is observed for other superconductors, and the observation has sparked considerable interest in the scientific community.

- Pencil-shaped organic molecules called "rod-coils," designed and synthesized to have half of the molecule rigid and the other half flexible, were discovered to exhibit unusual and important clustering mechanisms on several size scales. Because the building-block molecules are all oriented in the same direction, the film’s properties mirror those of the individual molecules, resulting in a film whose bottom surface is sticky and top surface is slippery. Such a film has many potential applications, for example, as an anti-ice coating on an airplane wing or an anti-blood-clot lining for artificial blood vessels.

- An atom-tracking STM was developed for direct measurement of surface dynamics.

- Magneto-optical imaging of magnetic vortices and transport currents in superconductors were accomplished.

- First principles quantum simulations of atomic structure, electronic conductance and dynamical fluctuations in metallic nanowires and carbon nanotubes have been performed. The results of these investigations allow deep insights into the physical nature of low dimensional materials systems and provide impetus for laboratory experiments aimed at the development of nanoscale devices and atomic scale switches.

- Prediction of multilayered semiconducting materials led to the production of a 30% efficient photovoltaic device now used in outer space.

- Recent three-dimensional simulations of turbulence, transport, and macroscopic stability in fusion plasmas have provided insight into the fundamental processes at work. For example, three-dimensional turbulence simulations have shown that zonal flows can lead to the formation of "transport barriers" in plasmas, thus dramatically reducing the loss of energy and particles.

- Understanding the physical mechanism responsible for high temperature superconductivity remains the outstanding problem in modern condensed matter physics. Recent experiments and theory indicate that, unlike common metals, electric currents in these superconductors are like rivers of charge, separated by atomic magnets present in the system. The picture resembles the stripes on a flag, which can be static or dynamic like a flag waving in the wind. Theory has shown that the interaction between the rivers of charge and the atomic magnets may be the key to understanding the exotic superconductivity in these materials.

- Traditionally, catalytic science has operated in two separate regimes: in solution (homogeneous), and on surfaces (heterogeneous). Each type of catalyst offers its own distinct advantages, but until recently attempts to interface the two centered on the use of easily studied homogeneous molecular catalysts to model putatively analogous phenomena on surfaces. Recently, has taken the opposite tack—attaching molecular catalysts to surfaces and exploiting the unique properties of each. This resulted in unique synergism, creating interesting new catalysts whose properties can be controlled through variations in the molecular catalyst and the supporting material. This new catalysis has the promise of creating new catalytic materials and generating fundamental knowledge that will result in a better understanding of catalytic phenomena.

- A combinatorial chemistry system has been devised for optimizing physical and chemical properties in which the chemical composition of a material can be changed, with each composition located at a point on a grid. The performance of each composition is then tested and the optimized composition can be selected easily and rapidly. Combinatorial chemistry is one of the important new methodologies to reduce the time and costs associated with producing effective, marketable, and competitive new substances. Scientists use combinatorial chemistry to create large populations of molecules, or libraries, that can be screened efficiently en masse. The field represents a convergence of chemistry and biology, made possible by fundamental advances in miniaturization, robotics, and receptor development.

- Techniques were developed to synthesize nanocrystals and to assemble them into useful structures. For example, a spray specialized atomization process produced a novel nanocrystalline composite powder with a crystallite size that matches that of a magnetic alloy. Adding the nanocrystals to the alloy produced stronger and cheaper high-strength, permanent magnets. The permanent magnet industry was worth $3.2 billion globally in 1995 and is predicted to reach $10 billion by 2010.

Adaptive Systems

Description, Objectives, and Research Performers

Research on complex, adaptive systems is the study of the behavior of macroscopic collections of individual units that are endowed with the potential to evolve in time. Their interactions lead to coherent behavior that can be described only at higher levels than those of the individual units. Hence, the whole is more than the sum of its components. For example, life forms survive by adapting to change. They evolve successfully or perish. These complex, self-organizing systems are adaptive, in that they don't just passively respond to events. Common underlying organizing principles are at work; these are the concern of fundamental studies in complexity. Two major research areas are concerned with understanding gene function and ecological processes. The research in these areas is conducted at national laboratories, universities and industrial firms.

Research on gene function provides information needed to understand the structure and function of the proteins and RNAs encoded by the human (and other) genome and to understand the nature of the regulatory networks that control expression of multiple genes in space and time. This information is fundamental to our understanding of the human genome and the genomes of microbes with broad applications in energy, the environment, medicine, agriculture, and industry.

Research on ecological processes advances scientific understanding of responses of terrestrial ecosystems and organisms to changes in climate and atmospheric composition, such as alterations in temperature and moisture and increases in carbon dioxide concentration. Objectives are to improve understanding of (1) the responses of terrestrial organisms and ecosystems to simultaneous changes in atmospheric composition and climate; (2) the causal mechanism or pathway of the responses and the biological and ecological processes controlling the responses; and (3) the extent to which the responses are manifested across different organizational (hierarchical) levels of terrestrial ecosystem components and processes of value to humans.

Research Challenges and Opportunities

Even the most primitive living organism controls the structure and function of its diverse products far better than the cleverest chemist. Understanding the structure, function, and regulation of genes at a genomic scale will be one of the great challenges in biology for the next several decades. In the past, questions of gene structure, function, and regulation have generally been addressed one gene at a time. With the availability, in the next several years, of sequence information for the entire human genome and for the genomes of many simple and complex organisms, this one-at-a-time approach will not keep pace with the availability of information on human genes. The national capabilities in genomics, structural biology, instrumentation and automation development, and the use of model organisms, such as the mouse, can be used to make important contributions to this new field of biology.

Knowledge of possible effects of climate and atmospheric changes on ecological systems has increased over the past decade and qualitative estimates of responses to such changes can be developed. However, our current ability to make quantitative predictions of the effects of

alterations in climate and atmospheric composition, such as increasing atmospheric carbon dioxide levels, on any particular ecosystem at any particular location is constrained by a limited understanding of many critical processes. Furthermore, the structure and functioning of terrestrial ecosystems are influenced by multiple climatic and non-climatic factors, the interactions of which are not always linear or additive. Further, very little research has studied the dynamic responses of ecosystems to simultaneous changes in multiple factors, particularly human-induced environmental changes to which ecosystems have not been previously subjected.

Research Activities

Research capitalizes on our understanding and the manipulability of the genomes of model organisms, including, for example, yeast, nematode, fruit fly, Zebra fish, and mouse, to speed understanding of human genome organization, regulation, and function. An important goal is to develop and use experimental systems and resources to characterize or analyze human gene function that match the speed of new gene discovery on a genomic scale. Research will closely coordinate with structural biology research that will develop high throughput technologies to provide information on gene structure.

Experimental and modeling studies on different types of ecosystems to investigate system responses to alterations in climate variables, atmospheric CO_2, ozone, and nutrient inputs. Studies using the Free-Air CO_2 Exposure (FACE) technology investigates the response of different types of ecosystems, including forest, grassland, desert, and croplands to elevated CO_2 and other environmental changes. A Throughfall Displacement Experiment is an experimental study of the response of a forest ecosystem to changing precipitation inputs. These experiments document responses to the experimental treatments, including the range of adjustments in physiological processes, above and below ground growth responses, and other structural and functional responses of the treated and reference or control ecosystems being studied. Results will be used to parameterize and test ecosystem response models that will be used to assess the consequences of human-induced environmental changes on terrestrial ecosystems.

Accomplishments

- Critical contributions in gene research include the development and application of flow cytometry, cDNA arrays, bio-chips for the parallel analysis of genes or proteins, algorithms to identify putative genes, strategies to induce and analyze mouse mutants, demonstration of gene regulatory mechanisms in DNA, cells and tissues, and tools and strategies for studying and characterizing human gene function in large blocks of DNA or fragments of chromosomes.

- Initial results of 7 long-term experiments on physiological and growth responses of forest, grassland and crop species and ecosystems show that increased CO_2 caused greater productivity and improved water use efficiency of these systems. A significant part of the productivity increase occurs below ground with roots, soil micro flora and the formation of soil organic matter.

- Findings from the Throughfall Displacement Experiment after six years show that changes in the seasonal timing of rainfall has a greater effect on the productivity of forest

ecosystems and carbon sequestration by forests than a uniform change in rainfall applied throughout the year.

Portfolio Summary

This portfolio area, "Complex Systems," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support or moderately support Complex Systems, including collective phenomena and adaptive systems. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these programs are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

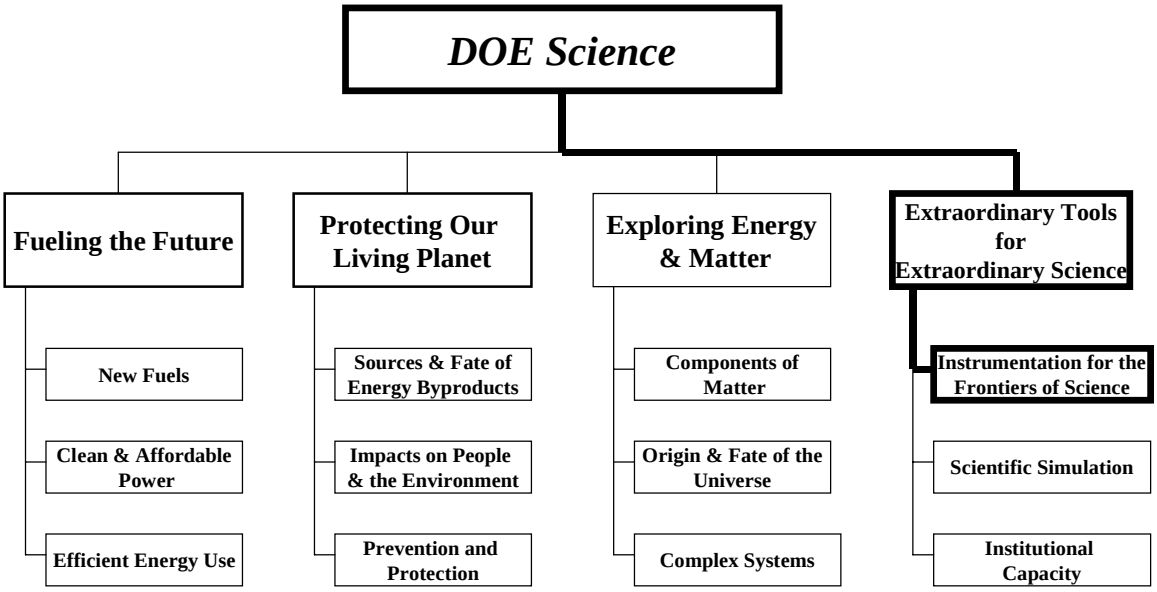
Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations
Applied Mathematics
Atomic, Molecular, and Optical Science
Catalysis and Chemical Transformations
Computer Science to Enable Scientific Computing
Energy Biosciences
Experimental Condensed Matter Physics
Fusion Physics Research on Alcator C-Mod
Fusion Physics Research on DIII-D
Fusion Physics Research on NSTX
General Plasma Science
Geosciences
High Performance Computer Networks
High Throughput DNA Sequencing
Materials Chemistry
Mechanical Systems, Systems Science, and Engineering Analysis
Neutron and Light Sources Facilities
Neutron and X-Ray Scattering
Photochemistry and Radiation Research
Physical Behavior of Materials
Plasma Theory and Computation
Resources and Tools for DNA Sequencing and Sequence Analysis
Scientific Computing Application Testbeds
Separations and Analysis
Structural Biology Research Facilities
Structure of Materials
Theory & Simulations of Matter, Engineering Physics
Understanding and Predicting Protein Structure
Understanding Gene Function

Moderately Supportive Core Research Activities
Advanced Computing Software and Collaboratory Tools
Advanced Fusion Materials Research
Advanced Medical Imaging
Analytical Chemistry Instrumentation
Chemical Energy and Chemical Engineering
Chemical Physics Research
Climate Change Technology Initiative (CCTI)
Engineering Behavior
Environmental and Molecular Sciences Laboratory (EMSL)
Experimental Fusion Physics Support
Experimental Plasma Research (Alternatives)
General Purpose Plant & Equipment (GPP/GPE)
General Technology: Accelerator R&D
Health Risks from Low Dose Exposures
Inertial Fusion Energy Research
Mechanical Behavior and Radiation Effects
Multiprogram Energy Lab Facilities Support (MELFS)
Oak Ridge Landlord
Production DNA Sequencing Facility
Radiopharmaceutical Development
Science Education Support

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Chapter 11
Instrumentation for the Frontiers of Science

Scientific Challenge: ***To provide research facilities that expand the frontiers of the natural sciences.***



Chapter 11

Instrumentation for the Frontiers of Science

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Conceiving and constructing the instrumentation of scientific research is at least as challenging as developing or proving any scientific theory and occupies a significant fraction of the research activity. A distinctive contribution of the Department of Energy and its predecessor agencies to science in the United States has been the construction and operation of leading-edge facilities for scientific research. Through universities and national laboratories, the Office of Science has maintained the United States' world leadership position in developing accelerators, reactors and accelerator-based neutron sources, synchrotron light sources, electron beam microcharacterization centers, plasma physics devices, supercomputers, and other special-purpose facilities such as the Joint Genome Research Institute, the Combustion Research Facility, and the William R. Wiley Environmental Molecular Science Laboratory.

These facilities enable scientists to acquire new knowledge required to achieve the Department's missions and, more broadly, to advance the U.S. scientific enterprise. The Office of Science continues to explore the frontiers of research through its stewardship of the most advanced scientific facilities in the world.

Accelerators for High Energy and Nuclear Physics

Description, Objectives, and Research Performers

Over the past 70 years each generation of accelerators has allowed scientists to answer a set of questions, make fundamental discoveries, and establish the questions to be answered by the next generation of accelerators. The Berkeley Bevatron, for example, was built in the 1950s to discover the anti-proton, long predicted by the Dirac Equation, and went on to become the discovery site for a host of new "particles." They were, in fact the first clues to the existence of quarks, but were not recognized as such until 1964 when the Omega-Minus particle was discovered at the Brookhaven AGS, a much more powerful accelerator than the Bevatron. The Bevatron itself was combined with a heavy ion linear accelerator in the 1970s to initiate the field of heavy-ion nuclear physics at intermediate energies. In more recent times, the discovery of the J/ψ meson and the tau lepton at SPEAR, the discovery of the W and Z bosons at the CERN Sp p S, and the discovery of the top and bottom quarks at the Fermilab Tevatron have established the Standard Model of particle physics. The discovery potential of these machines has been dramatically increased by colliding energetic beams of protons with one another or with anti-proton beams. This greatly increases the energy available for the creation of new particles, or new physics.

Alongside the development of high-energy proton accelerators has been the extension of electron accelerators to higher energies. The electron linac at the Stanford Linear Accelerator Center (SLAC) produced the second line of evidence for quarks as the basic constituents of neutrons and protons when researchers discovered the scaling phenomena in deep inelastic electron-proton scattering. SLAC has also been a pioneer in electron-positron collisions for particle physics with the SLAC Linear Collider (SLC), which accelerates electrons and positrons to 50 GeV and then brings them into collision with one another.

Today two new major nuclear physics accelerators are beginning operations: the Continuous Electron Beam Accelerator Facility (CEBAF) in New port News, Virginia; and the Relativistic

Heavy Ion Collider (RHIC) at Brookhaven National Laboratory. Each is a unique, world-class facility that promises new knowledge about the nature of nuclear matter and structure.

Research Challenges and Opportunities

High energy physics accelerators enable a wide range of inquiry: observing and understanding charge conjugation-parity (CP) violations; characterizing and determining the nature of neutrinos; observing rare particles in the collisions of protons and antiprotons, or of electrons and protons; measuring high energy phenomena in the universe from the early moments of the Big Bang and those observable today from distant stars and galaxies; and similar complex endeavors.

A specific challenge for research personnel at high energy physics accelerators is to build vertex and tracking systems that can withstand the high particle fluxes and high radiation exposure near beam pipes and interaction points. These conditions are expected with improved Fermilab Tevatron Run II-III upgrades and with the Large Hadron Collider (LHC) at CERN. Work on LHC detectors (ATLAS and CMS), BaBAR at SLAC, and Run II upgrades of CDF and D-Zero at Fermilab includes new developments in silicon pixel imagers, silicon vertex detectors, micro-strip gaseous detectors, radiation hard electronics for signal and data processing, and advances in superconducting magnet technology. Advances in science will require international collaboration in the construction and operation of future accelerators and detectors.

Researchers will continue to exploit the highly successful B-factory at SLAC, achieving luminosity beyond design for the asymmetric electron-positron collisions, reducing unwanted background radiation in the experimental zone, and maintaining the high level of operational readiness in order to further the experimental goals of the program. The linear accelerator will be operated to supply positrons and electrons simultaneously to the B-factory, End Station A, and the advanced accelerator physics experiments. Related challenges are the production of a highly polarized, extremely stable beam of particles to study Moller scattering in a hydrogen.

Other challenges for researchers using the high energy physics accelerators include using lasers, plasmas, and very high frequency radio sources to accelerate charged particles; applying advanced superconducting materials and new geometrics to build superconducting magnets for particle beam optical systems that operate with pole tip fields in excess of 16 Tesla; developing new high frequency, high power radio frequency sources; to develop higher current, higher brightness particle beam sources; formulating advanced software for computer modeling and simulation; and pushing forward theoretical charged particle beam dynamics and plasma physics as related to charged particle acceleration and control.

Nuclear physics accelerators are the sites for researchers to pursue various major challenges: investigating the quark/gluon substructure of nuclei: creating and understanding nuclei taken to their limits of deformation, excitation, and isotopic stability; understanding stellar burning and supernovae processes; performing nucleosynthesis of elements; studying the structure of nuclei that are far from beta stability, previously unavailable for experiment; investigating neutrino oscillation; and studying polarized ion nuclear reactions for unique high resolution spectroscopic information. A specific challenge is to provide electron and photon beams needed to probe various aspects of nucleon, meson, and nuclear structure. The nuclear physics accelerators will provide heavy ion beams needed to probe and understand the structure of nuclei and the various

phases of nuclear matter, and a variety of unstable and stable particle beams needed to probe various aspects of nuclear astrophysics and nuclear structure.

Research Activities

At Fermilab, experiments are ongoing to study neutrinos, B-mesons, known and new particles, and unusual states of matter. Fermilab has a large and well-equipped facility for assembling silicon microdetectors, a world-class data processing center, and an active group of theoretical physicists. It also serves as the host center for the U.S. efforts on the CMS detector and on the magnet development program for the LHC accelerator. Brookhaven National Laboratory serves as the host center for U.S. efforts on the ATLAS detector for the LHC accelerator. SLAC research facilities produce electrons and positrons, support the operation of the B-factory, and detect and measure the particles resulting from the collisionstherein. The Alternative Gradient Synchrotron (AGS) facility accelerates protons at 24 GeV, providing the world's highest intensity proton and kaon beams. These beams are used for forefront high energy and nuclear physics fixed target research aimed at understanding the fundamental structure of matter and energy.

Four major accelerators have either just started operations or will be operating by the year 2000: the CEBAF at the Thomas Jefferson National Accelerator Facility (TJNAF), which will open a new window on the role of quarks in nuclei; the RHIC, which will collide gold nuclei at 100 GeV per nucleon in search of the quark-gluon plasma which existed a hundredth of a second after the Big Bang; the Main Injector at Fermilab, which by raising the intensity of the beam by a factor of 5-10, will provide the opportunity to exploit the discovery of the top quark and search for other new particles such as a light Higgs; and the B-Factory at SLAC, which is studying the properties of the interaction that breaks the symmetry between matter and anti-matter, called charge-parity violation. Together, these leading-edge facilities will allow a significant improvement in the fundamental understanding of the nature of matter.

Modern physics research, in many cases, requires probe particle beams of great energy (billions and trillions of electron volts), very high currents, and exceptionally precise optical control. The science and technologies fundamental to building and operating such machines are highly specialized; ongoing R&D supports continual improvements in advanced computer modeling simulation and control software, and instrumentation for measuring particle beams.

Accomplishments

- Researchers at Stanford developed a germanium transition edge sensor that will be used for the search for galactic dark matter.

- The Tevatron collider is Fermilab's major accomplishment: 1000 superconducting magnets, all operating flawlessly, cooled by a 4-mile liquid-Helium system with refrigeration capability; and industrial-strength antiproton beams. During Run I of the Tevatron collider, which ended in 1996, there were about 1013 proton-antiproton collisions. Run I produced a tremendous amount of data, which led to the discovery of the top quark.

- The g-2 experiment at BNL usesthe largest superconducting magnet ever built, 15 meters in diameter, with field uniformity of 1 part per million along its circumference and a stability of 1 part per 10 million.

- The introduction of Lie Algebra techniques and symplectic (area preserving in phase space) requirements into the computation of accelerator and collider optical systems by a researcher at the University of Maryland enabled the modern million-turn simulation of storage rings that is now considered a major contribution to defining new machines.

- The demonstration of critical current densities of 5000 amperes per square centimeter in magnetic fields of 5 Tesla by a researcher at the University of Wisconsin shows the room for additional performance improvement over the current commercially available superconductor, which operates at about 3000 amperes per square centimeter.

- The invention of the laser wakefield and laser beat wave plasma acceleration concepts by researchers at the University of California at Los Angeles has opened up an entirely new means for charged particle acceleration.

- The proof-of-principle demonstration of the self-modulated, laser-driven plasma wakefield accelerator at accelerating gradients of greater than 100 GeV per meter and the laser driven plasma beat wave accelerator at accelerating gradients of 3 GeV per meter open a possible new path to ultra high gradient charged particle acceleration and the possible construction of accelerators of energy otherwise not economically feasible.

- The proof-of-principle demonstration of the particle driven plasma wakefield accelerator showed an alternative to lasers which does not require the development of optical channeling techniques to accelerate over long distances.

- Successful proof-of-principle demonstration of the Inverse Free Electron Laser shows that this device can provide very short (millionth of a meter) long bunches, and can probably be used as a quasi-linear, radiation-based transverse beam cooler.

- Successful proof-of-principle demonstration of inverse Cerenkov acceleration shows that by using a medium to control phase velocity of the laser, acceleration can be achieved at high gradients over centimeter distances.

- The successful application of NbTi superconductor technology in the construction of Fermilab's 1000 GeV Tevatroncontributed significantly to the industrialization of the underlying superconducting magnet technology later adapted for use in MRI imaging devices.

- The world's first full superconducting electron accelerator facility was completed at the Thomas Jefferson National Accelerator Facility (TJNAF). The high intensity, continuous wave, 4 GeV accelerator is being used to study the transition from the hadronic picture to the quark-based picture of nuclear physics.

- Major instrumentation has been built for the three experimental halls at TJNAF (with high resolution superconducting spectrometers, the CEBAF Large Acceptance Spectrometer (CLAS), a high momentum superconducting spectrometer, and a short-orbit spectrometer for measurement of short-lived reaction products.

- The Relativistic Heavy Ion Collider (RHIC) was completed and in FY1999 and is now being commissioned. The world's highest energy heavy ion collider facility will be used to search for the quark-gluon plasma, the state in which nucleons are melted into a soup of quarks and gluons—a state that only occurred previously at the instant after the Big Bang.

- A major upgrade and accelerator improvements to the pulse stretcher ring at the MIT Bates Linear Accelerator have recently been completed. The ring will be used to provide circulating continuous wave polarized beams for a new program of few-nucleon studies using internal gas targets.

- A new world-class Gammasphere detector is now in use to observe, with high precision, rare nuclear processes involving the emission of many gamma rays.

- The Sudbury Neutrino Observatory, located in a 7000-foot-deep mine, will be available for experiments in FY1999. The observatory will be used to resolve the question of the existence of a neutrino mass.

- At Oak Ridge National Laboratory, the Radioactive Ion Beam facility is enabling the first-time measurements of nuclear reactions that fuel the explosion of stars.

- The Next Linear Collider Test Accelerator (NLCTA) is used to demonstrate several technologies for use in high-frequency, microwave-driven linear accelerators and will be adapted as a gneral user facility for advanced accelerator physics and technology research.

- At the Multi-Particle Spectrometer Facility at Brookhaven National Laboratory scientists discovered the first definitive examples of exotic states: particles that are not totally composed of quarks.

- At the positive kaon spectrometer at Brookhaven National Laboratory scientists have recently discovered the rarest Standard Modelallowed decay ever observed at a branching ratio of 1 part in 100 billion. Another rare kaon experiment made the first observation of a decay that holds promise for determining a key quark mixing parameter of the Standard Model.

Light Sources and Neutron Beam Facilities for Natural and Life Sciences

Description, Objectives, and Research Performers

All science depends on advanced instrumentation to enable scientists to see structure and phenomena they have not observed before. The understanding of the behavior and properties of materials undergirds every major technology area. The sciences that focus on condensed matter, or materials research in general, are interdisciplinary, involving materials sciences, major areas of physics and chemistry, the earth sciences, biology, and medicine. Products of condensed-matter science, such as the transistor, the integrated circuit chip, and liquid crystal displays, have revolutionized our lives through their use in television, calculators, electronic watches, personal computers, appliances, autos, and innumerable other applications.

Light sources and neutron beam facilities improve our understanding of the fundamental interactions of photons, neutrons, electrons, and ions with matter, pending knowledge that can be used to design probes for materials sciences and related disciplines. Such information has made it possible for researchers to build the advanced machines and instrumentation necessary to create, manipulate, focus, and detect a large variety of beams of electromagnetic radiation and particles. As a result, new complex spectroscopic, scattering, and imaging techniques have been developed. These techniques further basic research in a wide variety of disciplines. Examples of investigations at the facilities include materials characterization, processing, and design; chemical kinetics, reaction dynamics, and reaction diagnostics; the molecular basis of geochemistry and environmental chemistry; and understanding materials under extremes of temperature and pressure for geophysical and earth sciences.

Research Challenges and Opportunities

Major challenges include understanding the physical mechanism that makes high temperature superconductivity possible and understanding giant or colossal magnetoresistance.

Photochemistry presents opportunities for altering chemical reaction pathways so that high volume industrial intermediates and specialty chemicals can be produced by less polluting processes. Research challenges include the spectroscopic investigation of natural photosynthetic systems at short times following the absorption of light to determine the nature of the excited electronic states involved in the energy conversion process.

Recently, scientists have used a Magnet Optical Trap (MOT) to trap atoms and form an atomic cloud known as a Bose-Einstein Condensate (BEC). A judicious use of multiple laser pulses can increase the number of atoms trapped in a MOT. A laser, other than those used to trap the atoms, could be used to modify the shape of the electron cloud in rubidium (Rb) atoms leading to an increase in number of trapped species. The modification in the shape of the electron cloud causes the atoms to attract rather than repel one another during a collision. In addition to the MOT's use as a testbed for quantum statistics, possible technological applications include developing an atom laser that can, conceptually at least, be used to "write" structures of atomic dimensions on a substrate, thus greatly reducing the size of microelectronic integrated circuits.

Progress in the biomedical sciences and in biotechnology increasingly depends upon understanding the relationship between the structure and function of biological molecules. Continued progress in meeting this demand will depend not only on efficient operation of the facilities but also on overcoming serious limitations in the capabilities of the best currently available instrumentation.

Research Activities

Synchrotron radiation can provide an intense source of light over a broad spectral range from the visible ultraviolet to the hard x-ray regions of the spectrum. The very precise properties of bremstrahlung, or synchrotron radiation, are used as a tool for other sciences, especially materials science, chemistry and biology. One of the best research tools available to science is the x-ray beam, a highly penetrating light ideally suited to a broad range of applications. Most of what we know about the three-dimensional arrangement of atoms in DNA, RNA, and viruses has come from x-ray research. X-ray light sources have also allowed scientists to conduct molecular-level examinations of ceramics and semiconductor materials, both of which are essential to the development of designer materials for new technologies.

The Stanford Synchrotron Radiation Laboratory (SSRL) was built in 1974 to take the intense x-ray beams from the Stanford Positron Electron Accelerating Ring (SPEAR) storage ring that was built for particle physics by the SLAC laboratory. Over the years, the SSRL grew to be one of the main innovators in the production and use of synchrotron radiation with the development of wigglers and undulators that form the basis of all third-generation synchrotron sources. The facility is now composed of 25 experimental stations and is used each year by over 700 researchers from industry, government laboratories, and universities. These include astronomers, biologists, chemical engineers, chemists, electrical engineers, environmental scientists, geologists, materials scientists, and physicists. The success of the SSRL and SPEAR has led to the development of new generations of light sources at other national laboratories:

- Advanced Light Source (ALS) at Berkeley is one of the world's brightest sources of ultraviolet light and soft x-rays, and a powerful source of higher energy x-rays, serving as an excellent probe of the electronic properties of atoms, molecules, surfaces, and condensed matter. It is also a powerful tool for determining the structure of macromolecules.

- National Synchrotron Light Source (NSLS) at Brookhaven provides intense focused light from the infrared through the x-ray region, probing crystal structure, molecular bonding, phase transitions, and many other properties germane to a wide range of sciences. It has 2,300 users from 350 institutions, including 50 corporations.

- Advanced Photon Source (APS) at Argonne is a third-generation hard x-ray source and one of only three of its kind in the world. It has 2000 users and covers a wide range of science and technology research from condensed matter physics and structural biology to lithography and micromachining.

Neutrons are a unique and effective tool for probing the structure of matter. Synchrotron light is an electromagnetic wave, but neutron beams behave as particles with mass which scatter off

various objects, but also like quantum-mechanical waves as they move through space. Because the neutron is uncharged electrically, it can penetrate deeply into materials and give precise information about the positions and motions of individual atoms in the interior of a sample—a tool invaluable in nondestructively measuring the internal strain in a material.

The neutrons are especially sensitive to the presence of certain isotopes of light elements, such as hydrogen, carbon, and oxygen, which are found in many important hydrocarbon and biological molecules; for example, the contrast between hydrogen and deuterium has revolutionized polymer physics. Beams of neutrons are particularly well suited for measurement of the positions as well as the fluctuations in these positions of atoms (phonons), and the structure (position and direction) of atomic magnetic moments in solids as well as the excitations in this magnetic structure (spin waves). Such studies allow physicists to take measurements leading to an understanding of phenomena such as melting, magnetic order, and superconductivity in a variety of solids.

Proton machines have not only advanced in energy, but also in the intensity of their beams. Typical currents have been in the microamp region, but some machines, in particular the LANSCE (Los Alamos Neutron Science Center) (formerly the LAMPF), accelerate a milliamp of protons to energies of 800 MeV. Originally built as a meson factory to produce pions and use them to study the properties of nuclei, this accelerator is now used in conjunction with the Proton Storage Ring (PSR) as a pulsed neutron spallation source for use in materials science and other fields for scientific and national security purposes.

A much more intense version of this machine, the Spallation Neutron Source (SNS), at the somewhat higher energy level of 1 GeV, will be built at Oak Ridge National Laboratory as a collaboration of five national laboratories. Initially the machine will operate at 1 milliamp, and eventually at 5 milliamp.

Argonne National Laboratory is also the location of the Intense Pulsed Neutron Source (IPNS), which uses protons from a linac plus rapid cycling synchrotron (the injector system for the late ZGS) and fires them into a depleted uranium source. It has been a highly innovative user facility for the study of materials from high-temperature superconductors through biological materials.

Reactors are well-established neutron sources. The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory is a light-water-cooled and -moderated reactor. It provides state-of-the-art facilities for neutron scattering and materials irradiation. The High Flux Beam Reactor (HFBR) at Brookhaven National Laboratory will be permanently closed. The nuclear research reactor was used for more than three decades by over 200 scientists annually for groundbreaking discoveries in physics and biology. The department is upgrading all of its neutron science facilities and is building the Spallation Neutron Source, which will help to alleviate the loss of HFBR.

Accomplishments

- The combination of intense, bright sources, tunability, and high photon energies has allowed vastly improved resolution and many orders of magnitude increases in signal, enabling the study of weak scattering from small samples and surfaces, novel

spectroscopies such as magnetic and inelastic scattering, real-time studies, and studies using the coherent properties of the beam. These experiments have forced scientists to rethink their basic understanding of semiconductors, metals, superconductors, alloys, composite materials, liquid crystals, surfaces and interfaces, magnetism, dynamic processes, elementary excitations, electronic structure, and factors controlling phase equilibrium.

- Experimental results from the APS include a new structural determination and biochemical analysis of the human fragile histidine triad (FHIT) protein, which derives from a chromosome that is commonly disrupted in association with cancers.

- Clifford G. Shull, long supported by the Department at Oak Ridge National Laboratory, was a co-winner of the 1994 Nobel Prize in physics for his work on experiments in which neutron waves fall on the crystal and scatter elastically (losing no energy) in a process called diffraction.

- The High Flux Isotope Reactor (HFIR) is the world's leading source of elements heavier than plutonium for research, medicine, and industry.

- Charge-coupled device detectors (CCDs) developed for structural-biology research, have become the standard detectors for protein crystallography. The program's Structural Biology Center at Argonne and Beamline 9 at SSRL were the first to routinely achieve sub-Ångstrom resolution of protein structures.

- High-precision area detectors for thermal neutrons have been developed based on helium 3 and on microelectronics. These detectors are essential for neutron scattering studies in structural biology and materials science, and are particularly well suited to neutron spallation sources.

Plasma and Fusion Energy Facilities

Description, Objectives, and Research Performers

Plasma and fusion energy sciences provide various facilities for the study of plasmas under various conditions and magnetic fields. Each of the three large fusion devices, as well as smaller facilities located at universities, provides a focus for participation by extended collaborative teams. Research is conducted at national laboratories, universities, and industrial firms.

Research Challenges and Opportunities

The main challenge of the National Spherical Torus Experiment (NSTX) is to integrate the research goals into a well-structured experiment. The spherical torus plasma regime is significantly distinct from most tokamak experiments. The magnetic fields are not large; the expected plasma parameters allow the exploration of new methods for starting the plasma and maintaining the necessary plasma currents. These innovative methods have been explored on small devices, but applicability to a larger system remains to be demonstrated. The potential for long-pulse operation, in which self-generated currents sustain the plasma, has been predicted.

High plasma pressures have been achieved on one small system. Calculations predict excellent confinement of the plasma in a spherical torus because of the unique plasma configuration. There are also predictions of improved (relative to conventional tokamaks) particle and power handling which would reduce requirements on plasma facing components.

The mission of the DIII-D national program is to establish the scientific basis for optimizing the tokamak approach to fusion energy production. The challenge is to improve the performance of heating and current drive tools such as electron cyclotron heating; the fueling tools; high speed pellet injectors; plasma facing components, such as carbon tiles for power exhaust; and plasma control systems. The associated challenge is to utilize these tools reliably and for long pulses. The R&D for the improvement of these hardware tools also advances the related engineering sciences.

The physics of plasma edge transport is enormously complicated because of the plethora of plasma, sheath, and atomic physics phenomena that can play a crucial role in the edge plasma. The behavior of power and particle exhaust depends on these phenomena. Understanding transport in high temperature plasmas, which are subject to many modes of micro- and macroscopic instability, represents another challenging task.

Alcator C-Mod is the newest, most advanced world-class tokamak, built to explore the physics of plasmas in a compact, high field environment. Alcator's high confining fields let researchers experiment with plasmas hotter and denser than those in machines of similar size. Alcator C was the first device to produce the density and confinement of hot plasma necessary for a useful fusion reaction. Alcator C-mod experiments help to increase our understanding of the principles governing the transport of particles and energy in high temperature plasmas. Divertor physics, plasma control, and plasma heating issues will continue to be explored in Alcator C.

Research Activities

The NSTX is being built as an innovative confinement concept in which the magnetic fields are not large. It began operating in 1999, with full scale experimental operations starting in 2000. The DIII-D facility is the largest operating magnetic fusion experiment in the United States that focuses on the advanced tokamak concept and has a 2.2 Tesla (T) field. By contrast the Alcator C-Mod facility is a high-field (8-9 T) user facility with currents much like DIII-D, namely 2.5 MA. Medium-grade experiments exploring alternative concepts are located at various universities, including the University of Wisconsin and UCLA.

Accomplishments

- During the past decade, the DIII-D program has made substantial contributions to the world fusion program on issues such as the optimum plasma shape, different modes of operations for higher performance plasmas and transport barrier formation, power exhaust plasmas, current drive by radio waves externally for continuous operation of fusion plasmas, and profile control for plasma stability.

- Alcator C-Mod has achieved high confinement that does not saturate at high density regimes as was feared in view of results of a previous generation of high field

experiments. This result bodes well for self-sustaining fusion reactions in compact high field tokamaks.

- Operation of high performance plasmas with radio frequency auxiliary heating alone has been established; this offers technological advantages over traditional neutral beam heating systems.

- Asymmetries in disruption halo currents first observed in Alcator C-Mod have become a critical consideration for the engineering design of future tokamaks. Alcator C-Mod engineers have also developed highly robust real-time algorithms for effective plasma control. The C-Mod approach has been adopted by other experiments.

Single-Purpose and/or Multi-Disciplinary Facilities

Description, Objectives, and Research Performers

DOE supports several different facilities of this type: *The William R. Wiley Environmental Molecular Science Laboratory (EMSL)* is a unique national scientific user facility. With over 100 leading edge instrument and computer systems in one facility, the EMSL provides users with the capability to undertake molecular-level research on environmental issues in an interdisciplinary environment. The EMSL is focused on basic research that can lead to significant improvements in the efficacy and cost of cleaning up contaminated environments, with emphasis on assisting the Department meet its responsibilities in environmental remediation and waste management. In 1999, over 800 users from academia, government laboratories, and industry used the EMSL instrument and computer systems.

Electron beam michrocharacterization centers provide essential tools for characterizing and analyzing the geometrical packing configurations of atoms in solids and crystals, defects and imperfections, and other properties of materials. They work at the scale of 1-2 Ångstroms; this scale determines the performance and detailed behavior of materials for many practical purposes. There are four Centers, located at Argonne, Lawrence Berkeley, and Oak Ridge National Laboratories, and the University of Illinois; they are networked and interfaced with one another. Serving over 1000 users annually, they provide world-class facilities for the physical sciences and engineering communities in scanning and transmission spectrometry and atomic force microscopy and related tools.

The Combustion Research Facility at Sandia-Livermore serves a broad array of university users exploring theoretical and experimental combustion systems. *The Materials Preparation Center* is a national user facility at Ames Laboratory. It provides unique, specialized equipment for the synthesis, processing, and analytical characterization of special materials, and it annually serves several hundred users from industry, universities, and other national laboratories. Centers that bring together scientists from different backgrounds working on common problems include the Centers for X-Ray Optics and Advanced Materials at Lawrence Berkeley National Laboratory, and the Surface Modification and characterization Facility at Oak Ridge National Laboratory, as well as the 100 Tesla Pulsed Field Magnet and the actinide photospectrometer at Los Alamos National Laboratory. Photochemistry and radiation facilities studying the capture of solar energy

at the molecular level are located at several national laboratories as well as one at the University of Notre Dame.

Research Challenges and Opportunities

Research challenges at the Combustion Research Facility are to improve theory and obtain confirmatory experimental measurements of the dynamics and spectroscopy of vibrationally and electronically excited species relevant to combustion systems. This will enable predictions of reaction rates under a wide variety of conditions, including high temperatures and pressures, energy transfer phenomena, and spectra for diagnostic probes.

Research Activities

Collectively, the electron beam microcharacterization centers embrace transmission, scanning, scanning-transmission, analytical, high and atomic resolution, high voltage, and environmental electron microscopies; atom probe and field ion microscopies; mechanical properties or microindentation instruments; atomic force microscopy; and nuclear microanlaysis. Dedicated capabilities include high spatial resolution x-ray energy dispersive chemical analysis for heavy elements, electron energy loss spectroscopy chemical analysis for light elements, extended x-ray absorption fine structure analysis, electron beam holography, atomic and sub-atomic spatial image resolution (with appropriate computer simulation interfacing and analysis), and various kinds of electron diffraction analyses. Various in situ capabilities allow real time experiments under extremes of high and low temperature, controlled gaseous environments, magnetic field-free and applied magnetic fields, various kinds of concurrent in situ particle irradiation, and controlled types and amounts of applied stress, all with a variety of multi-axis tilt-goniometric capabilities that have a critical effect on diffraction contrast imaging capabilities of crystal defects. The activities among these four user Centers are coordinated and interactive with one another via the Electron Beam Microcharacterization Collaboratory 2000 Telepresence Microscopy, which permits remote access and operation via the world wide web.

Accomplishments

- EMSL scientists have used cutting-edge fluorescence microscopy and spectroscopy to study the reaction dynamics of individual enzymes that degrade organic contaminants in real time and under different local environments. Using these tools, the change in the active site of a single biodegradative enzyme from an oxidized state to a reduced state can be observed.

- Research on nanoscale ice films has received national recognition because of its potential importance in research on solvation in aqueous solutions, cryobiology, and desorption phenomena in cometary and interstellar ices.

- EMSL scientists recently resolved a scientific controversy over the effect of the metal-coated fiber tip used in near-field scanning microscopy on fluorescence lifetimes by finding that fluorescence lifetime can be lengthened or shortened depending on the height of the aluminum tip above the molecule.

- Automated crystallographic texture mapping techniques have resulted in a thorough understanding of the role of grain boundary character on percolative current flow in high temperature superconductors.

- Determination of interfacial chemistry by state-of-the-art analytical electron microscopy techniques has clarified the operative toughening mechanisms in whisker-reinforced and self-reinforced ceramics.

- Microchemical composition analysis of the fine (Ångstroms) precipitates in stainless steels enabled development of new alloys with improved high-temperature creep resistance.

- Collective high-resolution electron microscopy, image simulations and microanalysis have been used to identify the major constituent in a new aluminum matrix mullite composite that is now being used in automotive applications.

- Modeling of a balance between interfacial and strain energies revealed that nanometer-sized precipitates in aluminum alloys could take only certain restricted or discrete sizes. This explanatory hypothesis was then used to optimize the behavior of hardened aluminum alloys used for automotive and aerospace applications.

- Recently scientists at the Combustion Research Facility have designed and refined a novel and elegantly simple experiment that allows the interaction of chemistry and turbulence to be examined in quantitative and verifiable detail for the first time. This experiment has unequivocally demonstrated an error in current models of basic combustion processes.

- Technologies that have been enabled as a consequence of the Materials Preparation Center include lead-free solder, freon-free refrigeration, recyclable lightweight automotive composite materials, nanocrystalline neodymium-iron-boron magnet alloys with matching crystallite and magnetic domain sizes, and quasicrystal coatings produced by plasma-arc-spray that have superior wear resistance and reduced surface friction.

Biological and Environmental Research Facilities

Description, Objectives, and Research Performers

Dedicated special facilities comprise key biological and environmental resources. Some are special beam lines and equipment stations at synchrotron light and neutron sources, and others are partially devoted to this area of research. Others are observation stations dispersed over large areas, taking regular readings of climatic conditions. Climate observation facilities are located in three climatologically significant regions, the largest concentration of instruments and facilities comprises the ARM Southern Great Plains Site – over 300 continuous data streams collected by instruments spread across an area of ~55,000 square miles.

Research Challenges and Opportunities

The accuracy of the data that will be produced through the Atmospheric Radiation Monitoring (ARM) program will be essential in bringing about resolution of the most important unresolved question in climate prediction, the role of clouds and solar radiation in climate. Furthermore, to enable decade-to-century climate prediction and understanding of climate variability, necessary to address long-term energy needs and distributions, measurement must be made over the span of a decade. In order for ARM to achieve its goals, its three sites must be maintained with both state-of-the-art instrumentation and data systems capable of transferring gigabytes of data with efficiency, accuracy, and timeliness. Not only are the three sites located in areas that have unique and critical climatological sites from the scientific viewpoint, but the climatologies also pose different challenges to the equipment.

Progress in the biomedical sciences and in biotechnology depends both on efficient operation of the facilities and on overcoming serious limitations in the capabilities of the best currently available instrumentation. Thus, a critical part of DOE stewardship includes the development and operation of experimental stations at the major facilities such as synchrotron light sources, neutron sources, and ultra high field mass spectrometers and nuclear magnetic resonance spectrometers, as well as research into new instrumentation such as detectors and data management and analysis systems.

Research Activities

Structural biology research facilities at the Argonne National Laboratory, Lawrence Berkeley Laboratory, and SSRL light sources investigate the sub-Ångstrom structures of proteins; other laboratories investigate PET scanning magneto encephalography and magnetic resonance imaging for single cell analysis on a fast time scale. At reactors located at MIT and McClellan Air Force Base, neutron beams are being used for clinical studies of boron neutron capture therapy. In the area of environmental studies, Field Research Centers are being established to study bioremediation of sites polluted with radionuclides. Other stations monitor carbon dioxide flow, atmospheric radiation, and water vapor through the ARM program. These efforts involve collaboration with other government agencies including NASA, NOAA, and the Department of Agriculture.

The Production Sequencing Facility (PSF) is devoted to the high-speed, automated sequencing of the human genome and is a key element of the DOE Joint Genome Institute. It is a high-throughput DNA sequencing factory that will utilize and integrate advances in sequencing technology and automation, drawing on the sequencing, automation and information management expertise of DOE National Laboratories and leading experts at universities. The PSF will begin operation in FY 1999.

The ARM infrastructure supports climate observatories in three climatic regions: the U.S. Southern Great Plains, the Tropical Western Pacific, and the North Slope of Alaska. These observatories gather data on clouds and on the local radiation budget, making total radiance as well as high resolution spectroscopic measurements of both the solar (incoming) and infrared (outgoing) atmospheric radiation. These data are used to improve the modeling of clouds and

radiation in General Circulation Models, the primary tool with which climate predictions are made.

Accomplishments

- Charge-coupled device detectors that were developed for structural-biology have become the standard detectors for protein crystallography. The program's Structural Biology Center at Argonne and Beamline 9 at SSRL were the first to routinely achieve sub-Ångstrom resolution of protein structures.

- The world's highest resolution and fastest 3D PET instrument was constructed.

- A nuclear medicine camera device for small animal and breast-specific imaging has been developed.

- Merging of PET's electronic radio tracer detectors, and magnetic resonance imaging's (MRI's) powerful magnetic fields has been accomplished.

- Development of a laser-based technology for single cell analysis enabled measurement of cellular enzyme substrates within a second time scale has been accomplished.

- High impact advances have been made in single atom and single molecule analysis schemes. To date, 52 R&D-100 Awards have been received for technologies developed by the researchers in the Measurement Sciences Program. Microscopic imaging of the contents of single cells using magnetic resonance tomographic methods has been demonstrated; this technology was applied to the analysis of tank waste sludges from the Savannah River Site, providing important practical insights on why a new treatment system had failed.

- More than 70 structures have been solved at the ALS Macromolecular Crystallography Facility, which has served more than 180 scientists in its first year of operation.

- The ARM North Slope of Alaska/Adjacent Arctic Ocean Site (NAS/AGO) is collecting data from a second site, inland from the Barrow site, at Atquasuk.

- The ARM Program atmospheric observatory at the Southern Great Plains site is being used for surface characterization and hydrology experiments by Department of Agriculture and NASA, for calibration and validation of NASA's Earth Observing System, and for storm studies conducted by the National Oceanic and Atmospheric Administration.

Computing and Computational Support

Description, Objectives, and Research Performers

Computing and the computational support essential to the success of all the programs is provided by state-of-the-art facilities and networking. These include the NERSC computing center at

Lawrence Berkeley National Laboratory and the ESNet, as well as Advanced Computing Research Facilities (ACRFs) at various DOE laboratories. In addition there are grand challenge efforts and collaboratory efforts involving the various programs.

Research Challenges and Opportunities

Massively parallel computers are difficult to program efficiently. New tools, as well as underlying system software support, are required to make this possible. Petascale data archives from advanced simulation as well as next generation experimental facilities require development of new technologies because current approaches do not scale. Other challenges include providing ultra high speed network access to massively parallel computers; development of tools to enable applications to effectively use network performance and status diagnostics; and integrating software produced by multiple groups into a single framework.

Research Activities

NERSC**,** located at Lawrence Berkeley National Laboratory, provides high performance supercomputers and associated software support for investigators supported by the Office of Science. The Center serves 2500 users working on about 700 projects; 35% of users are university based, 60% are in National Laboratories, and 5% are in industry.

ACRFs support advanced computational hardware testbeds for scientific application pilot projects and fundamental research in applied mathematics and computer science. ACRFs are located at Los Alamos National Laboratory (based on SGI/Cray Technology); Argonne National Laboratory (Intel-Based Clusters); and Lawrence Berkeley National Laboratory (SGI/Cray T3E and IBM-SP Technology). Related capital equipment such as high speed disk storage systems, archival data storage systems and high performance visualization hardware are also supported.

ESnet provides worldwide access to Office of Science facilities, including advanced light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, ACRFs, and other leading-edge science instruments and facilities. ESnet provides the communications fabric that links DOE researchers to one another and forms the basis for fundamental research in networking, enabling R&D in collaboratory tools and applications testbeds such as the national collaboratory pilot projects.

Supporting research aims to develop the most powerful and effective mathematical and computational tools for modeling, analyzing, and simulating complex phenomena in the core disciplinary and technology areas of DOE. This R&D applies the results of fundamental research in applied mathematics and computer science to an integrated set of tools that can be used by scientists in various disciplines to develop high performance scientific applications. Research is underway in computer science; high performance computer networks, their protocols, and methods for measuring their performance; software to enable high speed connections between high performance computers and both local area and wide area networks; software to make effective use of computers with hundreds or thousands of processors as well as computers that are located at different sites; large-scale scientific data management and visualization; and the underlying mathematical understanding and numerical algorithms to enable effective description and prediction of physical systems.

Accomplishments

- Various computational and communications tools have been completed: the Message Passing Interface (MPI-2) standard, development of Dynamic System Instrumentation tools and Applications Program Integration (API), Sandia University of Mexico Operating System (SUNMos) lightweight operating system kernal, Parallel Virtual Machine (PVM), and Globus to integrate geographically distributed computations and information resources.

- Tertiary tape storage systems have been integrated with distributed disk cache systems and object oriented database systems.

- The High Performance Parallel Interconnect (HiPPI) 6400 standard was completed.

- The Internet Engineering Task Force (IETF) accepted proposed differentiated services architecture, and these services were demonstrated.

- Software was interoperated by Argonne National Laboratory and Lawrence Livermore National Laboratory to build a framework that accelerated real application by a factor of more than 20.

- A modular electronic logbook framework was developed and widely deployed inside and outside DOE.

Portfolio Summary

This portfolio area, "Instrumentation for the Frontiers of Science," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support or moderately support Instrumentation for the Frontiers of Science, including accelerators for high energy and nuclear physics, light sources and neutron beam facilities for natural and life sciences, plasma and fusion energy facilities, single-purpose and multidisciplinary facilities, biological and environmental research facilities, and computing and computational support. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

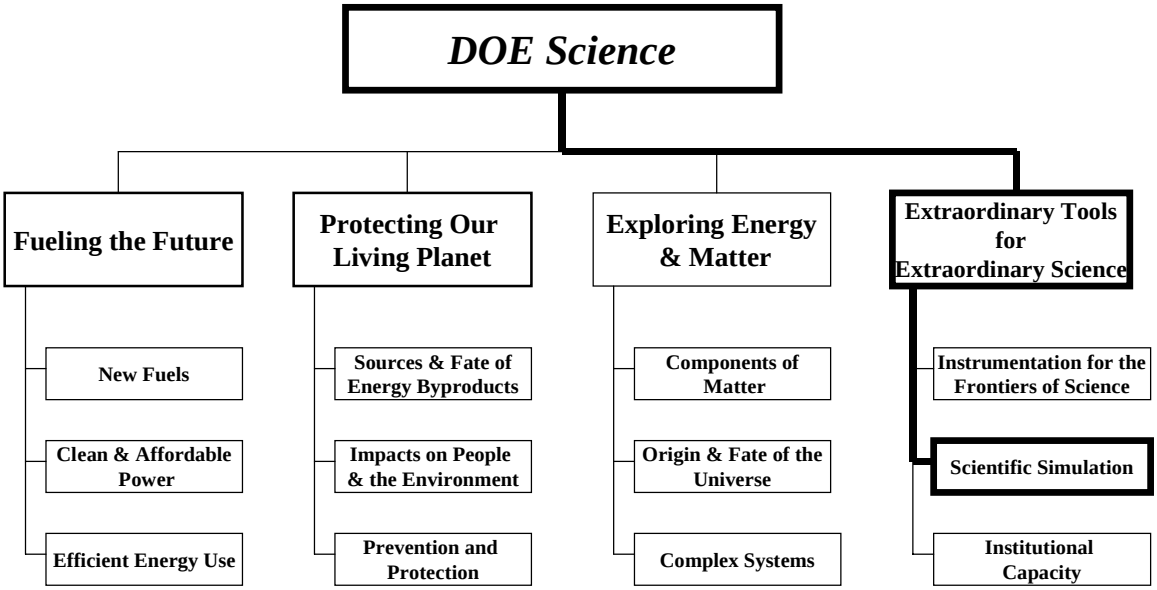
Strongly Supportive Core Research Activities
Adv. Particle Accelerator Concepts
Advanced Computing and Communications Facility Operations
Advanced Medical Imaging
Alcator C-Mod Facility Operations
Atmospheric Radiation Measurement (ARM) Program Infrastructure

Atomic, Molecular, and Optical Science Boron Neutron Capture Therapy Carbon Cycle Research Chemical Physics Research DIII-D Facilities Operations Ecological Processes Engineering Behavior Environmental and Molecular Sciences Laboratory (EMSL) Experimental Fusion Physics Support Experimental Plasma Research (Alternatives) Facility Operations: AGS Facility Operations: Fermilab Facility Operations: SLAC General Technology: Accelerator R&D General Technology: Detector R&D Heavy Ion Facility Ops. & Constr. High Performance Computer Networks Low Energy Facility Ops. & Constr. Medium Energy Facility Ops. & Constr. Natural and Accelerated Bioremediation Research Program Neutron and Light Sources Facilities NSTX Facility Operations Photochemistry and Radiation Research Production DNA Sequencing Facility Science Education Support Scientific Computing Application Testbeds Structural Biology Research Facilities Structure of Materials TFTR Facility Theory & Simulations of Matter, Engineering Physics
Moderately Supportive Core Research Activities Advanced Computing Software and Collaboratory Tools Catalysis and Chemical Transformations Chemical Energy and Chemical Engineering Computer Science to Enable Scientific Computing CP Violation - B-Meson System CP Violation - K-Meson System Electroweak Interactions Experimental Condensed Matter Physics General Purpose Plant & Equipment (GPP/GPE) Geosciences Hadron Spectroscopy Heavy Element Chemistry High Energy Physics Theory Materials Chemistry Mechanical Behavior and Radiation Effects Multiprogram Energy Lab Facilities Support (MELFS) Neutrino Mass and Mixing Neutron and X-Ray Scattering

Nuclear Structure & Astrophysics - Low Energy Nuclear Physics Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics Oak Ridge Landlord Particle Astrophysics & Cosmology Physical Behavior of Materials Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics Resources and Tools for DNA Sequencing and Sequence Analysis Search for Higgs & Supersymmetry Separations and Analysis Spin Structure of Nucleons Strong Interactions, Supersymmetry & Particles
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for eachCore Research Activity.

Chapter 12
Scientific Simulation

Scientific Challenge: ***To achieve computation and simulation as a critical tool in future scientific discovery.***



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Today computing is an integral part of virtually all scientific research. The World Wide Web was first developed by high-energy physicists to improve the scientific effectiveness of large, geographically distributed detector projects. As the price of microprocessors has fallen, computers have become an integral part of most advanced scientific instruments. In fact in many cases it would be impossible to accurately determine where the "instrument" ended and the "computer" began. Finally, high performance computers will be major instruments for scientific discovery in the coming years because they provide us with unique ways in which to view and analyze the world.

Simulation of physical systems on computers has been a critical component of DOE's (and its predecessor agencies') programs for 50 years. Driven initially by requirements for nuclear weapons design, computing is now critical to all of the missions of the Department. This has led the department to adopt a three-element approach to scientific simulation: (1) development of the advanced computer representations of physical systems of interest, (2) ultra high performance computational and communications facilities, and (3) development of the computational and software tools that enable scientists in the disciplines to make effective use of the computational and communications facilities. This approach is integral to the strategy for planning the future of scientific simulation in the Department. DOE's effective coupling of these elements has led to its leadership in the field.

Applications Software

Description, Objectives, and Research Performers

These activities focus on developing, testing, and using advanced computer software that realistically models physical processes. Significant portions of this activity are integrated into the management of all of the science programs of the Department. Examples of the types of applications software developed include global climate and ocean models, relativistic quantum chemistry software to understand the behavior of plutonium and uranium compounds in soil, and software to model fluid flow in combustion devices. These efforts have two common objectives: first, to increase the fidelity of the mathematical models of the physical phenomena under study; and, second, to find and implement ways of translating these models into computer code in ways that achieve very high efficiency and performance. This research is primarily conducted at national laboratories and universities.

Research Challenges and Opportunities

The rapid increase in computer speeds over the past decade has made possible applications with unprecedented fidelity to the natural world. It is now possible, for example, to create coupled atmosphere-land-ocean climate models with sufficient resolution to describe regional processes accurately. This change is opening up whole new fields of predictive computational inquiry. However, the applications developers must overcome significant challenges to take advantage of these resources. Both the range of physical phenomena that need to be included and the increased complexity of the next generations of computers will require large, interdisciplinary teams to develop and analyze the results of the next generation of scientific applications. In addition, the rate of change of the underlying computer systems implies that scientific software will have to be developed that is capable of being moved from one generation of hardware to the

next many times during its life. Finally, implementing the appropriate scientific models on the next generation of hardware with perhaps 10,000 processors will require discovering new ways to represent physical models on computers.

Overcoming these challenges will dramatically improve our ability to predict the behavior of physical systems through simulation. Prediction of mechanical properties of materials from microscopic structure; predictive design of low-emission diesel engines; and predictive models for complex systems such as fusion plasmas, pollutant flow through geological structures, and biological molecules are only a few of the advanced applications that will become possible. This type of computing will also enable the integration of optimization with predictive simulation and result in faster, more cost-effective design of processes ranging from particle accelerators for basic science to chemical processes in refineries.

Research Activities

The development of high performance applications software for scientific simulation is embedded in all of the scientific programs of the department. Current applications that use the National Energy Research Scientific Computing Center (NERSC) come from all of the areas supported by the Office of Science. In addition to the efforts which are embedded in the individual programs, DOE has conducted DOE-wide competitions such as the "Grand Challenge" component of DOE's High Performance Computing and Communications (HPCC) program. These projects represent partnerships between computer, computational, and other scientists to develop new techniques and make significant advances in the scientific state-of-the-art. The breadth of effort is demonstrated by the list of the current projects: global ocean and climate modeling; first principle micromechanical and continuum modeling of concentrated materials, methods, microstructure and magnetism; numerical tokamak turbulence project; particle physics phenomenology from lattice quantum chromodynamics; computational chemistry of nuclear waste characterization and processing, relativistic quantum chemistry of actinides; advanced modeling for next generation accelerator applications; grand challenge applications of high energy and nuclear physics data; high performance computational engine for the analysis of genomes; and supercomputer solution of massive crystallographic and microtomographic structural problems.

DOE's Defense Programs' Accelerated Strategic Computing Initiative (ASCI) also supports significant efforts in the development of software for weapons applications. Finally, detailed planning for future efforts in development of applications has occurred to understand, model, and predict the effects on the earth's global environment of atmospheric greenhouse gas emissions, with an emphasis on carbon dioxide; understand, model, and predict the behavior and properties of combustion processes and devices; and revolutionize basic scientific research by the application of teraflop computational resources in areas including materials sciences, structural genomics, high energy and nuclear physics, subsurface flow, and fusion energy research.

Accomplishments

- Software to model magnetism in metal alloys recently exceeded 1 teraflop in sustained performance.

- High resolution models for global ocean flow now accurately predict the path of the Gulf Stream as well as important large-scale ocean eddies, which transport energy from Africa across the Atlantic.

- State-of-the-art software, called NWChem, accurately models the chemistry of plutonium and uranium compounds.

Ultra High Performance Computational and Communications Facilities

Description, Objectives, and Research Performers

In addition to supporting the development of applications software, DOE supports many of the highest performance computing and communications facilities in the world. These facilities, just as other leading-edge facilities supported by the Department, have always had two roles: production of scientific results which are critical for the Department's missions and development of the hardware and software technologies that are required for the next generation of computational and communications facilities. These activities are supported at national laboratories, often in close partnership with U.S. firms that manufacture the computers and operate the underlying communications infrastructure.

Research Challenges and Opportunities

Operating computational and communications facilities at this scale presents significant challenges. Often technologies from a number of manufacturers need to be coordinated and made to interoperate to provide the end-to-end service that scientists require. Meeting these challenges requires a mix of skills from computer science, mathematics, data storage, computer hardware, and advanced software. In addition, because most of these facilities operate the most advanced technology currently available, they must develop much of the supporting software themselves because it is not available from commercial vendors. These facilities will enable scientific simulation to help solve pressing scientific questions related to the nuclear arsenal, climate prediction, combustion, and basic science in general.

Meeting these challenges will enable DOE to provide its researchers with the facilities they need to change science through simulation. In addition, DOE's facilities will become a model for facilities operated by universities and the commercial sector in much the same way that NERSC was the model for the NSF supercomputer centers.

Research Activities

Current examples of such computing research takes place at facilities such as NERSC, the computing facilities operated by the weapons laboratories, the advanced computing research facilities operated by the Office of Science at Argonne National Laboratory, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, and Oak Ridge National Laboratory, and more specialized computing resources such as the molecular sciences computing resource at Pacific Northwest National Laboratory's EMSL. In addition to computing facilities the Office of Science operates ESnet, a high performance network which links computational

and experimental facilities to users and is a critical component of the research infrastructure for the nation.

Detailed planning is currently underway for the next generation of computer and communications facilities that build on the experience of ASCI and move scientific simulation to the next frontier of multi-teraflop computing for future applications.

Accomplishments

- NERSC is the most powerful unclassified computer facility in the nation. At the recent Supercomputing Conference in Orlando, FL, the Gordon Bell Prize for highest performance computer application was awarded to a team that included NERSC. In addition, the three other finalists were from DOE computing facilities.

- NERSC's predecessor, the Magnetic Fusion Energy Computer Center, in partnership with other DOE facilities, pioneered interactive access to supercomputers. This approach, which allows users to observe their computer code while it is running, revolutionized the way in which supercomputers were used.

Computer Science and Enabling Technologies

Description, Objectives, and Research Performers

This program provides applications developers with the tools they need to make effective use of ultra-scale computer and communications facilities. These efforts provide mathematical algorithms and software, debugging and performance tuning tools, data management and visualization software, and tools to support collaboration over networks. These activities are carried out at national laboratories and universities with industrial partners in some cases.

Research Challenges and Opportunities

The complexity of the next generation of computer hardware as well as the massive amounts of data (millions of gigabytes) that they will generate pose significant challenges. A further challenge is coupling mathematicians and computer scientists into the next-generation applications teams effectively while maintaining strong, focused research programs in these disciplines.

These challenges must be met to enable scientists to take advantage of large-scale computation. Success here will make scientists across DOE more effective and productive. In addition, the computer science and enabling technology base that is produced will be critical for industrial acceptance of this scale of computing and promises to dramatically improve the productivity of U.S. industry and the viability of the U.S. high performance computing industry.

Research Activities

Activities include applied mathematics and areas of computer science that are relevant for high performance computing and remote access to facilities. Researchers in computer science and

enabling technology are working to overcome significant challenges and to enable important scientific applications. Software must be designed to support machines not only for the near future but for the next decade. Complex applications must be managed to incorporate more sophisticated physical models, using advanced numerical techniques, and begin to be combined into large-scale "simulation systems" that include the linkage of two or more previously stand-alone models (e.g., ocean-atmosphere- biosphere or fluid-structures-chemistry). Development and user environments must enable ubiquitous collaboration and distributed computing capabilities to support large interdisciplinary teams. Researchers must extract insight from, manage, and visualize petabyte scale data archives. Applications scientists and computer scientists and mathematicians must form more effective long-term collaborations.

All of these efforts must be balanced research, development, and deployment activities carried out in partnership with universities and commercial software and hardware vendors.

Accomplishments

- The DOE applied mathematics program, which was started by John von Neumann in the 1950s, has produced most of the high performance numerical linear algebra routines in the world.

- DOE pioneered remote access to supercomputers in the early 1970s and developed much of the underlying message-passing software that makes today's massively parallel computers useful.

- Phillip Colella, a mathematician at Lawrence Berkeley National Laboratory, received the 1998 Sidney Fernback Award from the Institute of Electrical and Electronics Engineers (IEEE) Computer Society, for his "outstanding contribution in the application of high performance computers using innovative approaches."

Portfolio Summary

This portfolio area, "Scientific Simulation," encompasses research from many research programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support, support, or provide facilities for applications software, ultra high performance computational and communications facilities, and computer science and enabling technologies. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these programs are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations
Advanced Computing Software and Collaboratory Tools
Applied Mathematics
Chemical Physics Research

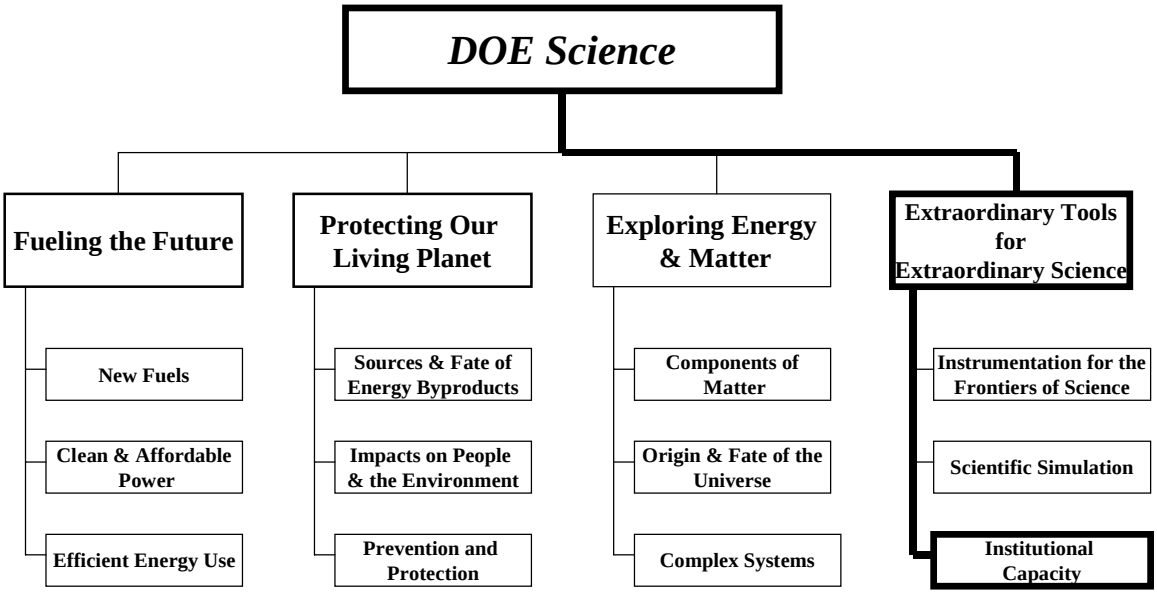
Climate Change Prediction Program
Environmental and Molecular Sciences Laboratory (EMSL)
Facility Operations: AGS
Facility Operations: Fermilab
Facility Operations: SLAC
General Technology: Accelerator R&D
Geosciences
High Energy Physics Theory
High Performance Computer Networks
High Throughput DNA Sequencing
Mechanical Behavior and Radiation Effects
Plasma Theory and Computation
Production DNA Sequencing Facility
Science Education Support
Scientific Computing Application Testbeds
Theoretical Nuclear Physics
Theory & Simulations of Matter, Engineering Physics
Understanding and Predicting Protein Structure

Moderately Supportive Core Research Activities
Adv. Particle Accelerator Concepts
Atmospheric Radiation Measurement (ARM) Program Infrastructure
Atmospheric Radiation Measurement (ARM) Program Research
Atomic, Molecular, and Optical Science"
Carbon Cycle Research
Computer Science to Enable Scientific Computing
CP Violation - B-Meson System
CP Violation - K-Meson System
Electroweak Interactions
Energy Biosciences
Engineering Behavior
Experimental Condensed Matter Physics
General Purpose Plant & Equipment (GPP/GPE)
General Technology: Detector R&D
Hadron Spectroscopy
Heavy Element Chemistry
Heavy Ion Facility Ops. & Constr.
Laboratory Technology Research and Advanced Energy Projects
Low Energy Facility Ops. & Constr.
Materials Chemistry
Mechanical Systems, Systems Science, and Engineering Analysis
Medium Energy Facility Ops. & Constr.
Multiprogram Energy Lab Facilities Support (MELFS)
Neutrino Mass and Mixing
Neutron and Light Sources Facilities
Neutron and X-Ray Scattering
Nuclear Structure & Astrophysics - Low Energy Nuclear Physics
Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics
Oak Ridge Landlord
Particle Astrophysics & Cosmology
Physical Behavior of Materials

Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics Search for Higgs & Supersymmetry Small Business Innovation Research (SBIR) Program Small Business Technology Transfer (STTR) Program Spin Structure of Nucleons Strong Interactions, Supersymmetry & Particles Structure of Materials
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for eachCore Research Activity.

Chapter 13
Institutional Capacity

Scientific Challenge: ***To strengthen the Nation's institutional and human assets for basic science and multidisciplinary research.***



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The Office of Science (SC) has statutory, programmatic, and institutional responsibilities to support the key components of the nation's science infrastructure. The Office provides institutional support for SC multiprogram national laboratories, funding for ES&H requirements at ten major SC laboratories, and line item construction funding to support general purpose infrastructure.

For science education purposes, support is provided for research at universities and colleges, and minority institutions, including graduate students and post-doctoral fellowships. A separate hands-on research internship program supports undergraduates and teachers at the Office of Science laboratories, during a summer or a semester.

SC is also responsible for broadening the scope of S&T performers in several ways. A Laboratory Technology Research (LTR) subprogram supports high risk, multidisciplinary research collaborations between SC laboratories and industry under Cooperative Research and Development Agreements (CRADAs). SC manages the DOE Small Business Innovation Research Program (SBIR), which uses small business to meet federal research and development needs, and the Small Business Technology Transfer (STTR) program, fostering small business collaborations with laboratories or universities to carry out research with commercialization potential. Targeted support through the DOE Experimental Program to Stimulate Competitive Research (EPSCoR) enhances the capabilities of eight states and the Commonwealth of Puerto Rico to carry out nationally competitive energy research, including close interactions and collaborative projects with DOE laboratories, and helps to develop science and engineering capabilities and expertise to meet future needs.

National Laboratory System

Description, Objectives, and Research Performers

The Office of Science has stewardship responsibility for five multiprogram national laboratories and five major program-dedicated laboratories. The SC programs have landlord responsibility for general purpose plant (GPP) and general purpose equipment (GPE) at all ten of these laboratories. Total funding for GPP/GPE for the multiprogram labs was $45.5M in FY 98 and $46.7M in FY 99.

SC programs support GPP funding (which is for small construction projects up to $5M) and GPE funding at Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge, and Pacific Northwest National Laboratories. The Director, Office of Science, is the cognizant Secretarial Officer responsible for the institutional management of these laboratories, including the Laboratory Institutional Planning, Work for Others, and Laboratory Directed Research and Development processes. Implementation of these and SC program responsibilities helps ensure effective support and advocacy of integrated safety management, performance-based management, nonprofit contract policy, and the laboratories operating as a system. Together these laboratories have more than 1000 buildings with 14.9 million gross square feet of space and a multitude of unique scientific facilities at an estimated replacement value of over $10.5 billion. The Office of Science helps ensure mission readiness of these laboratories and helps preserve the Federal investment in these unique institutions. The SC program funding at these laboratories ranges from 70% to 20% of total laboratory funding.

Total support of the infrastructure at Ames, Fermi, Princeton Plasma Physics Laboratory, Stanford Linear Accelerator Center, and the Thomas Jefferson Accelerator, where SC provides almost all of the funding, comes from the SC budget. Also, all the laboratories fund maintenance and ES&H from their overhead accounts, which come out of program budgets. These totaled $98M in FY97, based on functional cost data submissions from the labs.

The Office of Science also provides general infrastructure support for the backlog of general purpose facility needs at the aging SC laboratories at a level of about $20M per year. The Multiprogram Energy Laboratory Facilities Support (MELFS) program has been in existence since 1981 and has invested $421M in the SC multiprogram lab infrastructure over the years. Seventy percent of these funds ($280M) addressed utility and ES&H needs while 10% ($40M) provided new buildings. As a result, these investments have corrected life safety hazards, improved health standards, reduced environmental liabilities, provided reliable utility services, reduced operating costs, and improved operating efficiencies. The program also provides funds for Payment In Lieu of Taxes (PILT) to local governments for two SC laboratories (Argonne and Brookhaven) as allowed by the Atomic Energy Act of 1954.

Research Challenges and Opportunities

The MELFS program will continue to invest in the multiprogram energy laboratories, addressing line item construction funding for the highest environmental, safety, and health risk and the greatest return on investment. The program's focus is on ES&H needs, utilities, and rehabilitation or replacement of general lab and office space. The major purpose of these programs at all ten of SC's laboratories is to ensure that research at SC laboratories can be carried out with high efficiency and reliability, while ensuring the safety of the staff and public, and without adverse impact to the environment.

The principal ongoing challenge relating to the infrastructure investments is the prioritization of requirements so that the most critical ones can be addressed first. A secondary challenge is the overall funding level for line item construction. The need to improve reliability, reduce operating costs (e.g., maintenance and energy costs), increase productivity, and improve safety and environmental security at the SC laboratories is obvious. Investments today would, in fact, result in more funding for research in future years as operating costs are reduced.

Maintaining the integrity of laboratory programs requires continued focus especially on laboratory ES&H and infrastructure. The BNL Action Plan calls on the DOE Controller to lead the Department in establishing a corporate budget formulation and execution process for ES&H and infrastructure.

Accomplishments

- The Office of Science is piloting an integrated ES&H and infrastructure planning process linked to budget formulation and execution. This process will define expectations for the conduct of infrastructure management activities in FY 1998 and FY 1999 and will be used during the FY 2000 budget process at SC multiprogram laboratories.

Science Education

Description, Objectives, and Research Performers

The Office of Science programs are responsible for construction and operation of the cutting-edge national scientific user facilities that are indispensable to university, industry, and laboratory scientists in several research fields. The SC programs also fund over $1 billion in merit and peer reviewed research at the Department's R&D laboratories. This combination of facility and research support provides the healthy science and technology base at the major SC laboratories. This base is then used by all DOE programs and other agencies in carrying out research at the labs. The Office of Science supports about $500M of peer reviewed basic research in universities, plus an additional $500M for operating the SC scientific facilities at the laboratories for university science-based users. This represents the Department's largest program contributing to the university research base and to the education and training of graduate students and post docs produced by these universities to meet future scientific manpower needs.

The Office of Science program support of university and national laboratory research impacts about 3500 graduate students and post docs each year. This is an important DOE contribution to replenishing the overall U.S. scientific pool. It is also a source of new scientific talent for DOE and its laboratories. Thousands of university graduate students use SC's major scientific user facilities to perform their research. For example, out of the 2300 scientists that use the National Synchrotron Light Source each year, DOE supports 700 graduate student users, and other agencies support 550 more. SC programs also provide graduate fellowships to outstanding students in specific program areas.

The Basic Energy Sciences Program supports the EPSCoR at $6.8M per year at research universities and colleges in the designated eighteen states and the Commonwealth of Puerto Rico. This program also contributes to developing science and engineering manpower to help meet current and future needs. Particular emphasis is placed on exploiting the unique scientific and technical capabilities present at the DOE national laboratories to accomplish the objectives of the program. Close interactions result in establishing joint collaborative research projects between laboratory scientists and the EPSCoR state personnel. These projects, in turn, will lead to establishing nationally competitive scientific expertise at the home institutions of the EPSCoR states.

Research Challenges and Opportunities

A substantial number of highly capable students drop out of science programs in their sophomore and junior years in college. Hands-on research experience at the laboratories has proven effective in inspiring undergraduate students to remain in science. The undergraduate students and faculty work with researchers at the laboratories on DOE programs during the summer of their sophomore, junior or senior year or for a semester during their junior or senior year. The laboratory researcher often becomes a mentor to the student, and many students return to the laboratory for additional programs. The experiences vary by laboratory, and are tailored to the capabilities and needs of the students and teachers as much as possible. There are very few programs focused on undergraduates in S&T in the government. The SC base support for the

program helps to leverage program support for more than twice as many students each year. Support is provided mainly to undergraduates, graduate students, and post docs at DOE laboratories and, to a lesser extent, to pre-college students.

Accomplishments

- DOE has made a substantial contribution to the undergraduate education of over 100,000 students over the 40-year life of the predecessor program, and thousands of teachers and professors have also participated in the program over the past 10 years. The base support for the program helps to leverage program support for more than twice as many students as are directly supported each year.

- DOE carries out a National Science Bowl each year, which, since its inception, has had over 60,000 high school participants in regional tournaments, leading up the national finals in Washington, DC.

Broadening the Scope of S&T Programs

Increasingly, partnerships with universities, industry, and other laboratories characterize the programs carried out at SC laboratories. Industry scientists are a growing user group at the SC laboratories, both at the scientific user facilities, under work for others, and in formal collaborations and technology transfer partnerships with the laboratories. Thousands of industry scientists are currently carrying out research at laboratory user facilities. Many others are paying full cost recovery under Work for Others for the use of laboratory resources. Still others are participating in cost-shared Cooperative Research and Development Agreements. The Laboratory Technology Research (LTR) program is a separately funded research program cost-shared with industry partners for which SC is responsible. SC also manages the Department-wide Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs.

Research Challenges and Opportunities

The challenge is to expand the programs. There are many commendable applications for projects under the programs for every award the Department makes.

Research Activities

The LTR subprogram provides $16M to advance the fundamental science and technology at the SC laboratories toward innovative energy applications. The LTR subprogram supports high-risk, multidisciplinary research collaborations between the SC laboratories and private industry. The research portfolio emphasizes advanced materials processing and utilization, intelligent processes and controls, and sustainable environments. Such work leverages the resources of both partners, since each frequently has unique facilities and complementary expertise. The partners jointly bring technology research to a point where industry or DOE's technology development programs can pursue final development and commercialization. The LTR subprogram enhances opportunities to pursue technology research that is of value to industry, complements basic

research program goals, and seeks to enhance public benefit from investment in scientific research at the Office of Science laboratories.

In the DOE-wide SBIR program, 2.5% of the Department's extramural R&D budget, about $76M, is set aside for a competition among small businesses. The Department's technical program offices are responsible for identifying research challenges that (1) are suitable to the capabilities of technology-based small businesses and (2) are required to fulfill mission needs. The research challenges are published as technical topics in annual solicitations and encompass a wide range of scientific subject matter, from molecularly engineered nanoscale materials, to instrumentation and concepts for high-energy accelerators to advanced fuel injection concepts for hybrid electric vehicles.

The Small Business Technology Transfer (STTR) program is similar in structure to the SBIR program except that, in STTR, the small businesses must collaborate with a research institution (usually a national laboratory or a university) serving as a subcontractor. The Department sets aside 0.15% of its extramural R&D budget for competition among small businesses in this DOE-wide program. The responsibilities of the technical program offices are very similar to those in the SBIR program.

Accomplishments

- Since its inception in 1992, the LTR subprogram has won 19 R&D 100 Awards for the most technologically significant new products of the year and 17 Federal Laboratory Consortium Awards for Excellence in Technology Transfer.
- Each year, the Department selects approximately 200 SBIR awards from 1200-1500 applications.
- Each year, the Department selects approximately 15 STTR awards, from about 100-300 applications, to explore the feasibility of innovative concepts and development.

Portfolio Summary

This portfolio area, "Institutional Capacity," encompasses activities from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support or moderately support Institutional Capacity, including the national laboratory system, science education, and broadening the scope of S&T performers. Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities
Experimental Program to Stimulate Competitive Research (EPSCoR)
Fusion Physics Research on NSTX
General Purpose Plant & Equipment (GPP/GPE)
Laboratory Technology Research and Advanced Energy Projects
Multiprogram Energy Lab Facilities Support (MELFS)
Neutron and Light Sources Facilities

NSTX Facility Operations
Science Education Support
Small Business Innovation Research (SBIR) Program
Small Business Technology Transfer (STTR) Program

Moderately Supportive Core Research Activities
Adv. Particle Accelerator Concepts
Advanced Computing and Communications Facility Operations
Advanced Fusion Design
Advanced Fusion Materials Research
Alcator C-Mod Facility Operations
Carbon Cycle Research
CP Violation - B-Meson System
CP Violation - K-Meson System
DIII-D Facilities Operations
Economics of Global Climate
Electroweak Interactions
Experimental Fusion Physics Support
Experimental Plasma Research (Alternatives)
Facility Operations: AGS
Facility Operations: Fermilab
Facility Operations: SLAC
Fusion Physics Research on Alcator C-Mod
Fusion Physics Research on DIII-D
Fusion Technologies
General Plasma Science
General Technology: Accelerator R&D
General Technology: Detector R&D
Hadron Spectroscopy
Heavy Ion Facility Ops.& Constr.
Intertial Fusion Energy Research
Low Energy Facility Ops. & Constr.
Medium Energy Facility Ops. & Constr.
Neutrino Mass and Mixing
Nuclear Structure & Astrophysics - Low Energy Nuclear Physics
Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics
Oak Ridge Landlord
Particle Astrophysics & Cosmology
Plasma Technologies
Plasma Theory & Computation
Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics
Search for Higgs & Supersymmetry
Spin Structure of Nucleons
Strong Interactions, Supersymmetry & Particles
Theoretical Nuclear Physics

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.

Appendix
Budget Profiles

Appendix
Budget Profiles

This appendix contains the detailed information that underlies the quantitative aspects of our Portfolio Summary. The building blocks for this information are the Research Summary Profiles (RSPs), developed around individual Core Research Activities (CRAs), each with a unique title. In constructing the Profiles, DOE science programs were asked to organize their research into component pieces that could be "mapped" into the twelve science challenges. The goal was to reformulate (for purposes of this analysis) the programs in a way that would reveal additional insights into the makeup of the Department's portfolio—insights beyond those apparent through the budget structure alone. The result of this iterative effort is the 95 Research Summary Profiles, one for each Core Research Activity, for the Science Portfolio. In a number of cases, these Core Research Activities depict research areas at a finer level than they are presented in the President's FY 2000 Budget Request to Congress.

Each Research Summary Profile contains the following information, distributed across the two tables in this Appendix.

Title: a short descriptive title of the Core Research Activity.

Resources: an estimate of the amount for FY 98 and FY 99 that can be attributed to that Core Research Activity. Although the apportionment is subjective, all estimates collectively meet the budget control totals for science programs and for the overall science budget. *Because of the overlapping and highly crosscutting nature of the Science Challenges, multiple counting occurs across each Challenge.* ***Merely adding the resource estimates across science challenges will yield an estimate far in excess of the actual science budget.*** *The tables in this Appendix display how the Core Research Activities contribute to multiple challenges.*

B&R Links: reference to the contributing budget element(s)

Impacts: a subjective evaluation of the degree(s) to which the particular research item support(s) one or several of the twelve major science challenges. Impact is identified as either Strong (S) or Moderate (M). A blank indicates a lower impact.

Research Performers: an estimate of the distribution of resources by different categories of research performer: national labs, universities, industry, U.S. government, international/foreign.

Table A-1. Research Summary Impacts
(M=Moderately Supportive, S=Strongly Supportive)

					New Fuels	Clean and Affordable Power	Efficient Energy Use	Sources and Fate of Energy Byproducts	Impacts on People and the Environment	Prevention and Protection	Components of Matter	Origin and Fate of the Universe	Complex Systems	Instrumentation for the Frontiers of Science	Scientific Simulation	Institutional Capacity
	RSP Title	**FY 1999**	**FY 2000**	**FY 2001** Presd.Req	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
1	Structure of Materials	$24.111	$23.841	$26.778		M	S				M		S	S	M	
2	Engineering Behavior	$15.226	$15.521	$18.218		S	S						M	S	M	
3	Mechanical Behavior and Radiation Effects	$16.267	$16.570	$16.410		S	S						M	M	S	
4	Physical Behavior of Materials	$13.496	$14.065	$13.790		M	S						S	M	M	
5	Neutron and X-Ray Scattering	$24.891	$23.097	$23.441			M				M		S	M	M	
6	Experimental Condensed Matter Physics	$32.420	$33.313	$35.649		S	M				S		S	M	M	
7	Theory & Simulations of Matter, Engineering Physics	$15.124	$15.767	$18.876		M	M				S		S	S	S	
8	Materials Chemistry	$25.938	$25.796	$27.645	S		M				M		S	M	M	
9	Experimental Program to Stimulate Competitive Research (EPSCoR)	$6.815	$6.815	$9.815	M	M	M	M		M						S
10	Photochemistry and Radiation Research	$23.871	$23.351	$25.842	S		M	M			M		S	S		
11	Chemical Physics Research	$36.384	$31.191	$38.515		M	S			M			M	S	S	
12	Atomic, Molecular, and Optical Science	$11.018	$11.092	$12.123		M					S	M	S	S	M	
13	Catalysis and Chemical Transformations	$22.304	$21.857	$24.952	M		S	M					S	M		
14	Separations and Analysis	$13.950	$12.617	$14.617	M		M	M		S			S	M		
15	Heavy Element Chemistry	$6.642	$6.720	$7.376				S		M	M			M	M	
16	Chemical Energy and Chemical Engineering	$9.207	$9.009	$9.975	S	S	M						M	M		
17	Mechanical Systems, Systems Science, and Engineering Analysis	$17.476	$14.352	$17.767		M	S						S		M	
18	Geosciences	$22.792	$14.997	$15.205	S			S		M			S	M	S	
19	Energy Biosciences	$26.643	$25.041	$27.966	S			M	M	M			S		M	
20	Neutron and Light Sources Facilities	$394.551	$374.269	$569.783	M	M	M	M		M	M		S	S	M	S
N	Waste Management	$0.000	$0.000	$8.073												
21	Structural Biology Research Facilities	$15.471	$16.000	$20.500						M	M		S	S		
22	Understanding and Predicting Protein Structure	$11.429	$11.474	$15.390						M	S		S		S	
23	High Throughput DNA Sequencing	$46.000	$54.167	$54.052							S		S		S	
24	Resources and Tools for DNA Sequencing and Sequence Analysis	$38.119	$26.719	$28.218							S		S	M		
25	Radiopharmaceutical Development	$15.062	$14.413	$24.280						S			M			

					New Fuels	Clean and Affordable Power	Efficient Energy Use	Sources and Fate of Energy Byproducts	Impacts on People and the Environment	Prevention and Protection	Components of Matter	Origin and Fate of the Universe	Complex Systems	Instrumentation for the Frontiers of Science	Scientific Simulation	Institutional Capacity
26	Production DNA Sequencing Facility	$4.000	$4.000	$4.000							M		M	S	S	
27	Microbial Genomics	$10.633	$9.594	$18.362	S				M	S	S	S				
28	Analytical Chemistry Instrumentation	$5.844	$4.619	$5.849				S		S	M		M			
29	Health Risks from Low Dose Exposures	$12.316	$18.262	$11.682					S	M			M			
30	Advanced Medical Imaging	$26.490	$23.410	$16.390					M	S			M	S		
31	Understanding Gene Function	$22.788	$20.007	$24.221						M	M		S			
32	Boron Neutron Capture Therapy	$10.769	$11.290	$10.795						S				S		
33	Natural and Accelerated Bioremediation Research Program	$25.299	$25.173	$21.113					S	S	M			S		
34	Economics of Global Climate	$7.384	$6.844	$6.699				M	S							M
35	Environmental and Molecular Sciences Laboratory (EMSL)	$29.909	$28.823	$32.415	M		M		S	S	M		M	S	S	
36	Ecological Processes	$13.691	$11.924	$12.010					S					S		
37	Climate Change Prediction Program	$22.092	$23.845	$27.962				S	S						S	
38	Cleanup Research	$3.632	$3.383	$2.667	M	M		S	M	S						
39	Climate Change Technology Initiative (CCTI)	$13.135	$32.160	$35.761	S	S		S	S	S			M			
40	Carbon Cycle Research	$9.416	$15.483	$16.035				S	S					S	M	M
41	Atmospheric Sciences	$14.307	$12.641	$12.318				S	S							
42	Atmospheric Radiation Measurement (ARM) Program Research	$15.293	$15.997	$16.976				S	S						M	
43	Atmospheric Radiation Measurement (ARM) Program Infrastructure	$28.454	$27.371	$27.371				S	S					S	M	
44	Focused Health Research	$26.201	$17.797	$0.000					M	M						
45	Applied Mathematics	$22.564	$23.354	$33.054	S						S	S	S		S	
46	Computer Science to Enable Scientific Computing	$14.000	$14.000	$21.476	M	M	M		M		S	S	S	M	M	
47	High Performance Computer Networks	$7.420	$6.000	$7.500	M	M	M				S	M	S	S	S	
48	Advanced Computing Software and Collaboratory Tools	$13.841	$8.000	$14.600	M	M	S				S		M	M	S	
49	Scientific Computing Application Testbeds	$16.173	$8.732	$20.500			S				S	S	S	S	S	
50	Advanced Computing and Communications Facility Operations	$61.296	$55.996	$66.341		S	S		S		S	S	S	S	S	M
51	Laboratory Technology Research and Advanced Energy Projects	$18.148	$8.578	$11.963	M	M	S	M	M	S					M	S
52	Fusion Physics Research on DIII-D	$21.931	$23.025	$21.617		S							S			M
53	Fusion Physics Research on Alcator C-Mod	$7.775	$7.870	$7.367		S							S			M

					New Fuels	Clean and Affordable Power	Efficient Energy Use	Sources and Fate of Energy Byproducts	Impacts on People and the Environment	Prevention and Protection	Components of Matter	Origin and Fate of the Universe	Complex Systems	Instrumentation for the Frontiers of Science	Scientific Simulation	Institutional Capacity
54	Experimental Fusion Physics Support	$16.118	$16.666	$15.472		S							M	S		M
55	Fusion Physics Research on NSTX	$9.906	$12.874	$12.250		S							S			S
56	Experimental Plasma Research (Alternatives)	$18.980	$25.088	$23.665		S							M	S		M
57	Inertial Fusion Energy Research	$8.377	$15.281	$14.384		S							M			M
58	Plasma Theory and Computation	$22.666	$24.536	$27.536		S						S	S		S	M
59	General Plasma Science	$6.222	$7.964	$8.450		M						S	S			M
59a	TFTR Facility	$3.949	$13.422	$19.600										S		
60	DIII-D Facilities Operations	$29.065	$31.098	$29.255		S								S		M
61	Alcator C-Mod Facility Operations	$10.223	$10.657	$10.042		S								S		M
62	NSTX Facility Operations	$17.333	$15.506	$17.721		S								S		S
63	Plasma Technologies	$19.475	$12.085	$11.664		S										M
64	Fusion Technologies	$8.096	$9.222	$9.373		S			M							M
65	Advanced Fusion Design	$9.127	$5.271	$4.906		S			M							M
66	Advanced Fusion Materials Research	$6.840	$7.167	$6.804		S			M		M		M			M
67	CP Violation - B-Meson System	$14.324	$16.537	$16.862							S	S		M	M	M
68	CP Violation - K-Meson System	$7.519	$6.779	$6.912							S	S		M	M	M
69	Neutrino Mass and Missing Mass	$27.211	$31.848	$33.042							S	S		M	M	M
70	Search for Higgs & Supersymmetry	$65.000	$70.000	$70.000							S	M		M	M	M
71	Strong Interactions, Supersymmetry & Particles	$37.288	$41.322	$42.135							S	M		M	M	M
72	Electroweak Interactions	$38.718	$39.476	$40.252							S	M		M	M	M
73	Hadron Spectroscopy	$6.516	$8.188	$8.349							S	M		M	M	M
74	Spin Structure of Nucleons	$0.790	$0.886	$0.904							S	M		M	M	M
75	Particle Astrophysics & Cosmology	$4.633	$3.423	$3.490							M	S		M	M	M
76	High Energy Physics Theory	$29.194	$36.745	$37.467							S	M		M	S	
77	General Technology: Detector R&D	$13.835	$12.750	$11.565							S			S	M	M
78	Facility Operations: Fermilab	$219.711	$219.333	$219.447							S			S	S	M
79	Facility Operations: SLAC	$109.240	$118.271	$124.196							S			S	S	M
80	Facility Operations: AGS	$34.326	$4.994	$7.889							S			S	S	M
81	Adv. Particle Accelerator Concepts	$12.515	$13.140	$13.575							S			S	M	M
82	General Technology: Accelerator R&D	$42.706	$44.932	$49.191							S		M	S	S	M
83	Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics	$36.777	$36.962	$37.744							S	M		M	M	M
84	Medium Energy Facility Ops. & Constr.	$78.918	$76.900	$82.675							S	M		S	M	M

					New Fuels	Clean and Affordable Power	Efficient Energy Use	Sources and Fate of Energy Byproducts	Impacts on People and the Environment	Prevention and Protection	Components of Matter	Origin and Fate of the Universe	Complex Systems	Instrumentation for the Frontiers of Science	Scientific Simulation	Institutional Capacity
85	Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics	$54.028	$51.051	$51.333							S	S		M	M	M
86	Heavy Ion Facility Ops. & Constr.	$103.547	$116.203	$126.757							S	S		S	M	M
87	Nuclear Structure & Astrophysics - Low Energy Nuclear Physics	$22.998	$23.998	$24.193							S	S		M	M	M
88	Low Energy Facility Ops. & Constr.	$9.310	$8.941	$9.120							S	S		S	M	M
89	Theoretical Nuclear Physics	$15.640	$15.675	$18.155							S	S			S	M
90	Science Education Support (X)	$4.500	$4.500	$6.500	M	M	M	M	M	S	M	M	M	S	S	S
91	General Purpose Plant & Equipment (GPP/GPE)	$46.590	$47.178	$53.847	M	M	M	M	M	M	M	M	M	M	M	S
92	Multiprogram Energy Lab Facilities Support (MELFS)	$21.260	$21.255	$23.219	M	M	M	M	M	M	M	M	M	M	M	S
93	Small Business Innovation Research (SBIR) Program	$76.850	$55.744	$58.849	M	M	M	M	M	M					M	S
94	Small Business Technology Transfer (STTR) Program	$4.611	$3.344	$3.525	M	M	M	M	M	M	M				M	S
95	Oak Ridge Landlord	$0.000	$11.800	$10.711	M	M	M	M	M	M	M	M	M	M	M	M

X — $4.5m of Science Education activities are being funded out of the SC Program Direction account in FY 1999 and FY 2000 and $6.5m in FY 2001.

Table A-2. Research Summary Funding by Research Performer

						Percent of Funding by Research Performer				
	B&R	RSP Title	FY 1999	FY 2000	FY 2001 Pres. Req.	Lab	Univ	Ind	Gov	For
1	KC020101	Structure of Materials	$24.111	$23.841	$26.778	68	32	0	0	0
2	KC020105	Engineering Behavior	$15.226	$15.521	$18.218	91	9	0	0	0
3	KC020102 KC020104	Mechanical Behavior and Radiation Effects	$16.267	$16.570	$16.410	78	21	1	0	0
4	KC020103	Physical Behavior of Materials	$13.496	$14.065	$13.790	76	24	0	0	0
5	KC020201	Neutron and X-Ray Scattering	$24.891	$23.907	$23.441	77	23	0	0	0
6	KC020202	Experimental Condensed Matter Physics	$32.420	$33.313	$35.649	77	23	0	0	0
7	KC020203 KC020204 KC020205	Theory & Simulations of Matter, Engineering Physics	$15.124	$15.767	$18.876	85	15	0	0	0
8	KC0203	Materials Chemistry	$25.938	$25.796	$27.645	72	26	1	1	0
9	KC0205	Experimental Program to Stimulate Competitive Research (EPSCoR)	$6.815	$6.815	$9.815	5	95	0	0	0
10	KC030101	Photochemistry and Radiation Research	$23.871	$23.351	$25.842	50	49	0	1	0
11	KC030102	Chemical Physics Research	$36.384	$31.191	$38.515	80	19	0	1	0
12	KC030103	Atomic, Molecular, and Optical Science	$11.018	$11.092	$12.123	42	58	0	0	0
13	KC030201	Catalysis and Chemical Transformations	$22.304	$21.857	$24.952	55	41	0	4	0
14	KC030202	Separations and Analysis	$13.950	$12.617	$14.617	68	32	0	0	0
15	KC030203	Heavy Element Chemistry	$6.642	$6.720	$7.376	95	5	0	0	0
16	KC030204	Chemical Energy and Chemical Engineering	$9.207	$9.009	$9.975	55	45	0	0	0
17	KC0401	Mechanical Systems, Systems Science, and Engineering Analysis	$17.476	$14.352	$17.767	41	53	1	5	0
18	KC0403	Geosciences	$22.792	$14.997	$15.205	48	50	2	0	0
19	KC06	Energy Biosciences	$26.643	$25.041	$27.966	9	88	1	2	0
20	KC020401	Neutron and Light Sources Facilities	$394.551	$374.269	$569.783	100	0	0	0	0
N		Waste Management	$0.000	$0.000	$8.073					
		TOTAL BES	**$759.126**	**$720.091**	**$962.816**					
21	KP110101	Structural Biology Research Facilities	$15.471	$16.000	$20.500	90	10	0	0	0
22	KP110101 KP110401	Understanding and Predicting Protein Structure	$11.429	$11.474	$15.390	76	24	0	0	0
23	KP110301	High Throughput DNA Sequencing	$46.000	$54.167	$54.052	90	10	0	0	0
24	KP110301	Resources and Tools for DNA Sequencing and Sequence Analysis	$38.119	$26.719	$28.218	21	79	0	0	0
25	KP140101 KP140102 KP140104	Radiopharmaceutical Development	$15.062	$14.413	$24.280	40	60	0	0	0
26	KP110301	Production DNA Sequencing Facility	$4.000	$4.000	$4.000	100	0	0	0	0
27	KP110201	Microbial Genomics	$10.633	$9.594	$18.362	40	60	0	0	0
28	KP140201	Analytical Chemistry Instrumentation	$5.844	$4.619	$5.849	90	10	0	0	0
29	KP110202 KP110401	Health Risks from Low Dose Exposures	$12.316	$18.262	$11.682	51	44	0	0	5

						Percent of Funding by Research Performer				
30	KP140102 KP140103 KP140104 KP140106 KP140107	Advanced Medical Imaging	$26.490	$23.410	$16.390	50	50	0	0	0
31	KP110201 KP110301 KP110401	Understanding Gene Function	$22.788	$20.007	$24.221	80	20	0	0	0
32	KP140105	Boron Neutron Capture Therapy	$10.769	$11.290	$10.795	46	54	0	0	0
33	KP130101	Natural and Accelerated Bioremediation Research Program	$25.299	$25.173	$21.113	50	50	0	0	0
34	KP12040	Economics of Global Climate	$7.384	$6.844	$6.699	35	65	0	0	0
35	KP130103	Environmental and Molecular Sciences Laboratory (EMSL)	$29.909	$28.823	$32.415	100	0	0	0	0
36	KP120301 KP120302	Ecological Processes	$13.691	$11.924	$12.010	40	60	0	0	0
37	KP120101 KP120102	Climate Change Prediction Program	$22.092	$23.845	$27.962	49	45	0	5	1
38	KP130102 KP130105	Cleanup Research	$3.632	$3.383	$2.667	56	36	8	0	0
39	KC02 KC03 KC0403 KC06 KP120202 KP120203 KP110201	Climate Change Technology Initiative (CCTI)	$13.135	$32.160	$35.761	(W)	(W)	(W)	(W)	(W)
40	KP120202 KP120203	Carbon Cycle Research	$9.416	$15.483	$16.035	30	65	0	0	0
41	KP120201	Atmospheric Sciences	$14.307	$12.641	$12.318	63	37	0	0	0
42	KP120103 KP120104	Atmospheric Radiation Measurement (ARM) Program Research	$15.293	$15.997	$16.976	44	33	2	19	1
43	KP120103	Atmospheric Radiation Measurement (ARM) Program Infrastructure	$28.454	$27.371	$27.371	99	0	1	0	0
44	KP110201 KP120203 KP120402 KP140107	Focused Health Research	$26.201	$17.797	$0.000	(W)	(W)	(W)	(W)	(W)
		TOTAL BER	**$427.734**	**$435.396**	**$445.066**					
45	KJ0101	Applied Mathematics	$22.564	$23.354	$33.054	65	35	0	0	0
46	KJ0101	Computer Science to Enable Scientific Computing	$14.000	$14.000	$21.476	75	25	0	0	0
47	KJ0102	High Performance Computer Networks	$7.420	$6.000	$7.500	75	25	0	0	0
48	KJ0101 KJ0102	Advanced Computing Software and Collaboratory Tools	$13.841	$8.000	$14.600	65	35	0	0	0
49	KJ0101 KJ0102	Scientific Computing Application Testbeds	$16.173	$8.732	$20.500	60	40	0	0	0
50	KJ0102	Advanced Computing and Communications Facility Operations	$61.296	$55.996	$66.341	100	0	0	0	0
51	KJ02 KJ03	Laboratory Technology Research and Advanced Energy Projects	$18.148	$8.578	$11.963	100	0	0	0	0
		TOTAL ASCR	**$153.442**	**$124.660**	**$175.434**					

						Percent of Funding by Research Performer				
52	AT501020	Fusion Physics Research on DIII-D	$21.931	$23.025	$21.617	35	6	59	0	0
53	AT501030	Fusion Physics Research on Alcator C-Mod	$7.775	$7.870	$7.367	25	75	0	0	0
54	AT5010101 AT501080 AT501070 ATGI	Experimental Fusion Physics Support	$16.118	$16.666	$15.472	40	47	4	9	0
55	AT501501	Fusion Physics Research on NSTX	$9.906	$12.874	$12.250	80	14	5	0	1
56	AT501502	Experimental Plasma Research (Alternatives)	$18.980	$25.088	$23.665	45	54	0	1	0
57	AT501503	Inertial Fusion Energy Research	$8.377	$15.281	$14.384	94	2	2	2	0
58	AT5020	Plasma Theory and Computation	$22.666	$24.536	$27.536	47	38	15	0	0
59	AT5030	General Plasma Science	$6.222	$7.964	$8.450	15	69	0	16	0
59 a	AT5501	TFTR Facility	$3.949	$13.422	$19.600	100	0	0	0	0
60	AT5502	DIII-D Facilities Operations	$29.065	$31.098	$29.255	9	0	91	0	0
61	AT5503	Alcator C-Mod Facility Operations	$10.223	$10.657	$10.042	5	95	0	0	0
62	AT5505 AT5508	NSTX Facility Operations	$17.333	$15.506	$17.721	100	0	0	0	0
63	AT601030	Plasma Technologies	$19.475	$12.085	$11.664	44	53	3	0	0
64	AT601040	Fusion Technologies	$8.096	$9.222	$9.373	68	31	1	0	0
65	AT601050	Advanced Fusion Design	$9.127	$5.271	$4.906	49	40	9	0	2
66	AT6020	Advanced Fusion Materials Research	$6.840	$7.167	$6.804	86	13	1	0	0
		TOTAL FES	**$216.083**	**$237.732**	**$240.106**					
67	KA04	CP Violation - B-Meson System	$14.324	$16.537	$16.862	25	75	0	0	0
68	KA04	CP Violation - K-Meson System	$7.519	$6.779	$6.912	25	75	0	0	0
69	KA04	Neutrino Mass and Missing Mass	$27.211	$31.848	$33.042	25	75	0	0	0
70	KA04	Search for Higgs & Supersymmetry	$65.000	$70.000	$70.000	25	75	0	0	0
71	KA04	Strong Interactions, Supersymmetry & Particles	$37.288	$41.322	$42.135	25	75	0	0	0
72	KA04	Electroweak Interactions	$38.718	$39.476	$40.252	25	75	0	0	0
73	KA04	Hadron Spectroscopy	$6.516	$8.188	$8.349	25	75	0	0	0
74	KA04	Spin Structure of Nucleons	$0.790	$0.886	$0.904	25	75	0	0	0
75	KA04	Particle Astrophysics & Cosmology	$4.633	$3.423	$3.490	25	75	0	0	0
76	KA04	High Energy Physics Theory	$29.194	$36.745	$37.467	25	75	0	0	0
77	KA04	General Technology: Detector R&D	$13.835	$12.750	$11.565	50	50	0	0	0
78	KA02	Facility Operations: Fermilab	$219.711	$219.333	$219.447	100	0	0	0	0
79	KA02	Facility Operations: SLAC	$109.240	$118.271	$124.196	100	0	0	0	0
80	KA02	Facility Operations: AGS	$34.326	$4.994	$7.889	100	0	0	0	0
81	KA04	Adv. Particle Accelerator Concepts	$12.515	$16.140	$13.575	35	22	40	3	0
82	KA04	General Technology: Accelerator R&D	$42.706	$44.932	$49.191	100	0	0	0	0
		TOTAL HEP	**$663.526**	**$668.624**	**$685.276**					
83	KB0101	Quark/Gluon Substructure of Nuclei - Medium Energy Nuclear Physics	$36.777	$36.962	$37.744	55	45	0	0	0
84	KB0102	Medium Energy Facility Ops. & Constr.	$78.918	$76.900	$82.675	84	16	0	0	0
85	KB0201	Nuclear Structure/Dynamics ... Phase Trans. - Heavy Ion Nuclear Physics	$54.028	$51.051	$51.333	65	35	0	0	0
86	KB0202	Heavy Ion Facility Ops. & Constr.	$103.547	$116.203	$126.757	100	0	0	0	0
87	KB0401	Nuclear Structure & Astrophysics - Low Energy Nuclear Physics	$22.998	$23.998	$24.193	54	46	0	0	0

						Percent of Funding by Research Performer				
88	KB0402	Low Energy Facility Ops. & Constr.	$9.310	$8.941	$9.120	100	0	0	0	0
89	KB0301	Theoretical Nuclear Physics	$15.640	$15.675	$18.155	42	58	0	0	0
		TOTAL NP	**$321.218**	**$329.730**	**$349.977**					
90	Program Dir.	Science Education Support (X)	$4.500	$4.500	$6.500	70	30	0	0	0
91	Cross Cut	General Purpose Plant & Equipment (GPP/GPE)	$46.590	$47.178	$53.847	100	0	0	0	0
92	KG	Multiprogram Energy Lab Facilities Support (MELFS)	$21.260	$21.255	$23.219	100	0	0	0	0
93	KM0000	Small Business Innovation Research (SBIR) Program	$76.850	$55.744	$58.849	5	10	85	0	0
94	KN0000	Small Business Technology Transfer (STTR) Program	$4.611	$3.344	$3.525	25	15	60	0	0
95	AH99	Oak Ridge Landlord	$0.000	$11.800	$10.711					
		Total All Other	**$153.811**	**$143.821**	**$156.651**					
		GRAND TOTAL	**$2,694.940**	**$2,660.054**	**$3,015.326**					

W — This Research Summary includes new program elements and as such the distribution of these research funds has yet to be decided.
X — $4.5m of Science Education activities are being funded out of the SC Program Direction account in FY 1999 and FY 2000 and $6.5m in FY2001.