

## SCIENCE: SIGNIFICANT PERFORMANCE RELATED TO ADVANCING SCIENTIFIC UNDERSTANDING

*Science Strategic Goal: To protect our national and economic security by providing world-class scientific research capacity and advancing scientific knowledge.*



*Technician at the B Factory's huge BABAR detector system at the Stanford Linear Accelerator Center. BABAR is a 1,200 ton detector system that can sift through the 238 million beam crossings that will occur every second in the B Factory and analyze the three to four events that can best be studied for charge-conjugation/parity.*

Basic scientific research in the physical sciences is one of the foundations for economic growth and national security in this country. Achievements and the public benefits in public health, telecommunications, supercomputing, to name just a few examples, are dependent upon progress in the physical sciences. No one has made this connection any clearer than former National Institutes of Health Director Harold Varmus, when he said, "Medical advances may seem like wizardry. But pull back the curtain, and sitting at the lever is a high-energy physicist, a combinational chemist or an engineer. Magnetic resonance imaging is an excellent example. Perhaps the last century's greatest advance in diagnosis, magnetic resonance imaging, is the product of atomic, nuclear and high-energy physics, quantum chemistry, computer science, cryogenics, solid state physics and applied medicine."

The Department's Office of Science is one of the primary government sponsors of basic research in the United States, and leads the Nation in supporting the physical sciences in a broad array of research subjects in order to improve our Nation's energy security, and to address issues ancillary to energy, such as climate change, genomics, and life sciences.

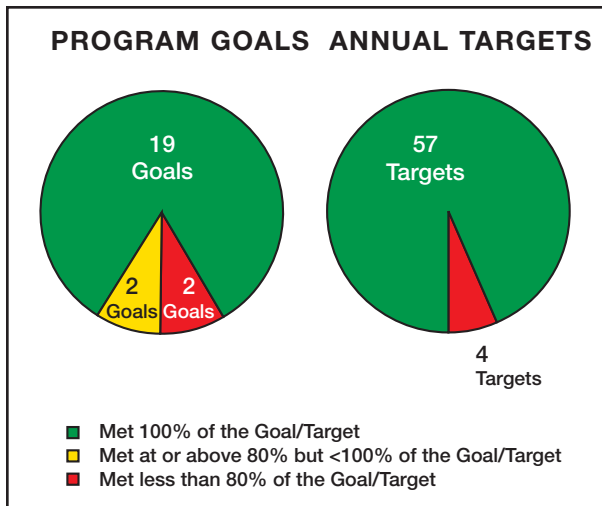
An important component of the Department's science activities is its operation and management of ten national laboratories and 27 scientific user facilities, including x-ray and optical

light sources, supercomputers, fusion devices, and particle accelerators across the country. The suite of user facilities plays a vital role in the Nation's science and technology portfolio, annually drawing over 17,000 users from universities, industry, and government.

The Office of Science also makes substantial investments in the Nation's research universities. Each year nearly \$800 million is invested in over 280 universities through the competitive grants program. Each project is selected on the basis of merit review for quality and relevance. Performance is tracked by the responsible program manager. Results are published in the open literature in the appropriate, peer reviewed journal such as: Physics Review Letters, Science, and Nature.

By the very nature of Office of Science research efforts, and the enormous scale at which these issues must be addressed, a robust and diverse scientific research capability has been developed. The President's affirmation of the importance of Federal investments in science and technology continues an unbroken line of support by our Nation's leaders for the sciences that stretches back 56 years – a line of support that parallels the history of the Office of Science and its predecessors.

### FY 2003 PERFORMANCE AT A GLANCE



### COSTS AT A GLANCE

SCIENCE STRATEGIC GOAL COSTS (IN MILLIONS)		
GPRA PROGRAM	FY 2003 Costs	FY 2002 Costs
General Goal 5: World-Class Scientific Research	\$3,068	\$2,830
<b>TOTAL COSTS</b>	<b>\$3,068</b>	<b>\$2,830</b>

**GENERAL GOAL 5 - WORLD-CLASS SCIENTIFIC RESEARCH CAPACITY:** Provide world-class scientific research capacity needed to: ensure the success of Department missions in national and energy security; advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences; and provide world-class research facilities for the Nation's science enterprise.

The common thread woven through all of the Department's activities is science, and Office of Science basic research underpins the Department's applied technology programs through strategic investments that fuel discoveries in materials sciences, chemistry, plasma science, plant sciences, biology, computation and environmental studies.

The Office of Science sponsors leading edge basic research in physics and other areas that extend the frontiers of knowledge and discovery. Through these investments in basic research, the Office of Science is tackling some of the most challenging scientific questions of the 21st century.

The remainder of this section is structured to present relevant performance information in the following areas:

- Exploring Matter, Energy, Space, and Time (encompassing Science Program Goals SC 1-1 and SC 2-1);
- Harnessing the Power of Our Living World (encompassing Science Program Goals 3-1 and 3-2);
- Advancing the Basic Science for Energy Independence (encompassing Science Program Goals 4-2 and 7-4);
- Delivering Computing for the Extremes of Science (encompassing Science Program Goal 5-2); and
- Bringing the Power of a Star to Earth (encompassing Science Program Goal 6-1).

### EXTERNAL FACTORS

The following external factors could affect our ability to achieve this goal:

- **Scientific and Technical Talent:** The prospect of the insufficient scientific and technical talent in certain key subfields, now and in the foreseeable future, threatens our ability to meet Departmental missions.
- **Balanced Investments in Science:** The growing interdependencies in research create several issues of balance that need to be incorporated into funding decisions. The Department is actively working with the other research agencies to maximize the impact and balance of the Federal research and development portfolio.

## PERFORMANCE RESULTS

### Exploring Matter, Energy, Space, and Time:

*Understand the unification of fundamental particles and forces, the structure of nuclear matter, the processes of nuclear astrophysics, and the mysterious forms of unseen energy and matter that dominate the universe; search for possible new dimensions of space; and investigate the nature of time itself.*

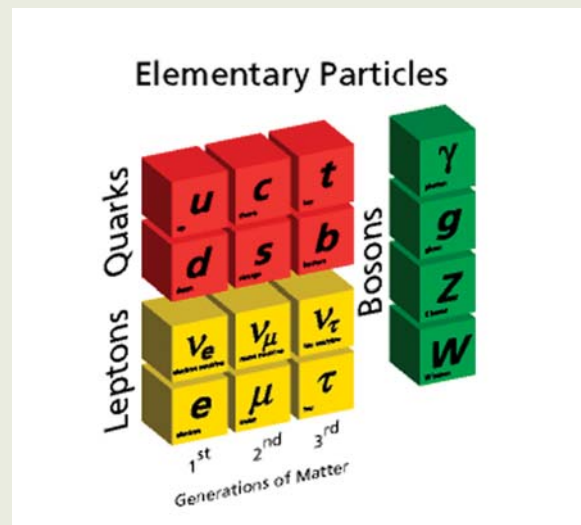
The physical sciences have answered many of the basic questions that puzzle humankind. Led by great scientists like Galileo, Newton, Einstein, and Heisenberg, we have learned much about the vast reaches of space and time and the varied forms of matter and energy found in the universe. In the early 20th Century, we learned that the universe is huge, contains billions of galaxies like our Milky Way, and is expanding. We also learned about quantum behavior and the structure of matter and energy, a profound advance with many practical benefits. In just the last few decades, physicists have discovered that all matter is composed of only 12 types of fundamental particles — ten of which were discovered by the Department's Office of Science research programs — which interact by means of four basic forces.

As impressive as these discoveries are, we are continuously humbled by what we do not know or do not fully understand. For example, we learned recently that the expansion of the universe is accelerating, not slowing down as we had thought. This astonishing discovery is attributed to a mysterious new form of energy—called “dark energy”—that accounts for about 70 percent of the energy density of the universe. The next largest fraction, about 25 percent, is made up of another mysterious substance dubbed “dark matter.” Only five percent of the universe can be detected by humans, with the stars we see at night making up less than one percent.

The study of high energy physics, also known as particle physics, grew out of nuclear and cosmic ray physics in the 1950's that used a relatively new technology, particle accelerators. Today, that technology has advanced so that particle accelerators produce exquisitely controlled beams with energies of trillions of electron volts

## QUARKS, LEPTONS, AND BOSONS

Physicists currently believe there are three types of basic building blocks of matter: quarks, leptons, and bosons. Quarks and leptons make up everyday matter, which is held together by bosons. Each boson is associated with a force. The photon, the unit of the electromagnetic force, holds the electron to the nucleus in the atom. The way these particles combine dictates the structure of matter.



and intense enough to melt metal. While science has revolutionized our understanding of how the universe works, elements of the technology have helped transform other fields of science, medicine, and even everyday life. This area of science will be remembered as one of the highlights of the history of the late 20th century.

In Fiscal Year 2003, High Energy Physics Program continued its work in areas that may well change our understanding of the universe, focusing on unique opportunities for discoveries in physics, utilizing the world-class facilities built for this purpose. In particular:

**Program Goal SC 1-1:** Exploit U.S. leadership at the energy frontier by conducting an experimental research program that will establish the foundations for a new understanding of the physical universe.

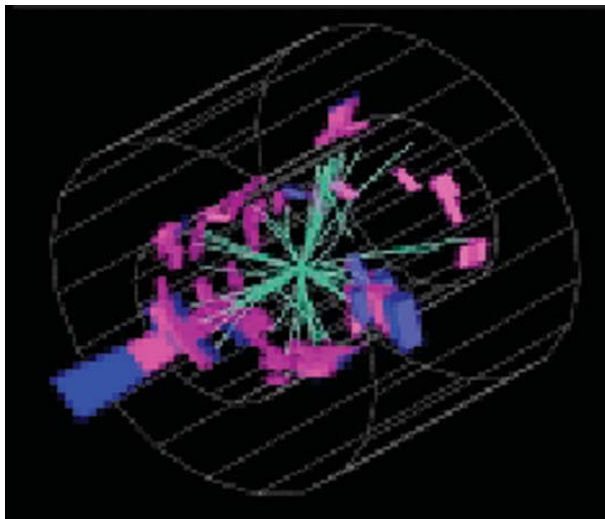
The discovery of the quark structure of matter was a scientific advance that may be compared to the discovery of the atomic nucleus in the early 20th century. This new knowledge is part of the Standard Model, our

theory of the fundamental particles and their interactions. The Standard Model proposes that an interaction called the Higgs Field, permeates the universe and gives mass to elementary particles.

Finding evidence of the Higgs Field has been a principal goal of high energy physics research for years, with searches underway at accelerator facilities around the world. This Program Goal focuses on the use of the Tevatron proton-antiproton collider at the Fermi National Accelerator Laboratory to continue its contribution towards the discovery of the Higgs Field by studying the very heavy top quark, which was discovered at this laboratory.

**Target SC 1-1a:** Deliver integrated luminosity as planned 225 inverse picobarns to Collider Detector at Fermilab and D-Zero at the Tevatron.

**Assessment and Commentary:** This target was met. The integrated luminosity delivered to the Collider Detector and D-Zero Detector was 240 inverse picobarns, exceeding the target. Luminosity is a measure of particle interaction and increasing it improves the chance of observing new particle reactions involving quarks and



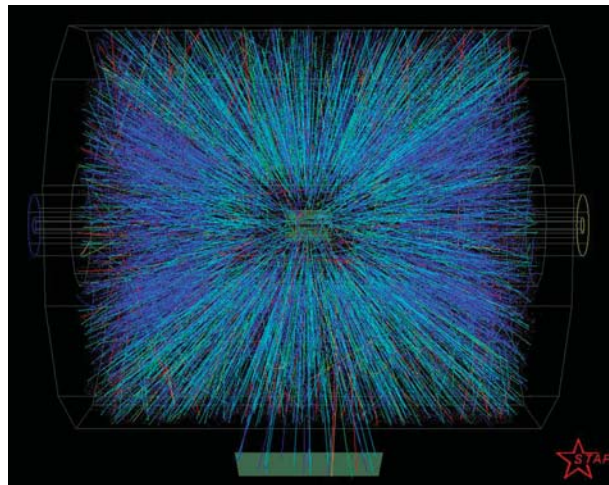
*Simulation of a Higgs boson event as it might appear in a detector at Fermilab.*

other fundamental building blocks of matter.

Nuclear physics began by studying the structure and properties of atomic nuclei as assemblages of protons and neutrons. Great benefits, especially to medicine,

emerged from these efforts. But today, nuclear physics extends from the quarks and gluons that form the sub-structure of the once-elementary protons and neutrons, to the most dramatic of cosmic events—supernovae. At its heart, nuclear physics attempts to understand the composition, structure, and properties of atomic nuclei.

**Program Goal SC 2-1:** Determine the structure of nucleons in terms of bound states of quarks and gluons. Measure the effects of this structure on the properties of atomic nuclei.



*View of the first full energy collisions between two gold ions at the Brookhaven National Laboratory Relativistic Heavy Ion Collider captured by the STAR detector. The tracks indicate paths taken by thousands of sub-atomic particles produced in the collision.*

Protons and neutrons, collectively called nucleons, are the building blocks of nuclear matter and thus form the heart of all atoms in the universe. But nucleons are themselves composed of quarks bound together by gluons, the “force carriers” (called bosons) that transmit the strong nuclear force. The nucleus is an ideal system to study the strong interaction, which can be described by a process called Quantum Chromodynamics.

To understand nucleon structure, one area of nuclear physics research is to probe quark confinement inside the nucleon. Specifically, although protons and neutrons can be separately observed, their quark constituents cannot be, because they are permanently confined inside the nucleons. While the mechanism of quark confinement is qualitatively explained by Quantum Chromodynamics, a quantitative understanding remains one of mankind’s great intellectual challenges.

**Target SC 2-1b:** Map out the strange quark contribution to nucleon structure using the G-Zero Detector, utilizing the high intensity polarized electron beam developed at the Thomas Jefferson National Accelerator Facility as elements of the electron beam program.

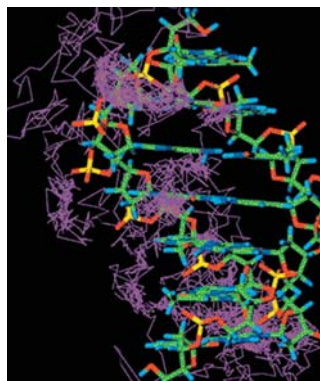
**Assessment and Commentary:** This target was met. The Thomas Jefferson National Accelerator Facility research program using the G-Zero Detector to measure the strange quark content was initiated in Fiscal Year 2003. Data from the initial engineering run has been analyzed and indicate the existence of a new kind of matter that contains five quarks rather than the two or three that make up all matter presently observed. This may provide vital information on how quarks and gluons interact to form nuclear matter.

### Harnessing the Power of Our Living World:

*Provide the biological and environmental discoveries necessary to clean and protect our environment, offer new energy alternatives, and fundamentally alter the future of medical care and human health.*

Over billions of years of evolution, Nature has created life's machinery from molecules, microbes, and complex organisms to the biosphere, all displaying remarkable capacities for efficiently capturing energy and controlling precise chemical reactions. The natural, adaptive processes of these systems offer important clues to designing solutions to some of our greatest challenges.

In Fiscal Year 2003, the Department continued its efforts to reveal the mechanisms and genetic secrets by which microorganisms develop, survive, and function in different environments. These studies will ultimately lead to our ability to manipulate matter at the micro, nano, and molecular scales; and to model and predict biological and environmental interactions on a regional and global basis. Such capabilities will provide unprecedented opportunities to forge new pathways to energy production, environmental management, and medical diagnosis and treatment.



*Molecular dynamics simulation of DNA with a sodium counter-ion.*

### Program Goal SC 3-1:

Determine, compare, and analyze DNA sequences of microbes and other organisms that will underpin development of biotechnology solutions for clean energy, carbon sequestration, and environmental cleanup.

The 21st century may be called the “biological century” – an era when advances in biology, spurred by achievements in genomic research, including the sequencing of the human genome, will bring revolutionary and unconventional solutions to some of our most pressing and expensive challenges in health, energy, the environment, and national security.

The Department began the program to map the human genome when others felt it would be impossible, and used the Department's national laboratories' expertise in the physical sciences and computing to develop the techniques that allowed its completion two years ahead of schedule. We can now map two billion base pairs a month, or two human genomes a year. The impact of DNA mapping is well documented. Gene therapies for cystic fibrosis, sickle cell anemia, diabetes and cancer are something we read about often now.

#### Biology + Nanotechnology for Energy

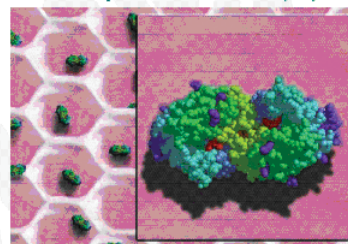
**Applications**—*Engineered protein machines (from microbes) with extended operating times can be embedded in synthetic nanomembranes to:*

*Produce* hydrogen from water for fuel cells

*Clean up* toxic wastes

*Filter* noxious fumes before venting air to the atmosphere

*Experiments show enhanced biocatalytic lifetimes*



In Fiscal Year 2003, this knowledge is being applied in novel ways by the Office of Science to attempt to use genetic techniques to harness microbes to eat pollution, create hydrogen, and absorb carbon dioxide. The possibilities are tremendous — to be able to understand how living organisms interact with and respond to their environments so that we will be able to use biology to produce clean energy, remove excess carbon dioxide from the atmosphere, and help clean up the environment.

**Target SC 3-1d:** Produce draft DNA sequences of more than 30 microbes vital to future United States energy security and independence, carbon sequestration, and environmental cleanup.

**Assessment and Commentary:** The draft DNA sequencing of more than 30 microbial organisms of relevance to the Department's missions of energy carbon sequestration and environmental cleanup were completed. These microbes are important because they have the potential to provide a clean source of energy, remove greenhouse gasses from the atmosphere and sequester or clean up environmental contaminants.

**Program Goal SC 3-2:** Establish the scientific foundation for determining a safe level of greenhouse gases and aerosols in the atmosphere by resolving or reducing key uncertainties in predicting their effects on climate, and provide the foundation to predict, assess, and mitigate potential adverse effects of energy production and use on the environment.

We are confronted with changes to the Earth's climate and have made progress in measuring and modeling these shifts. This is no simple matter, given the complex interactions of air, land, and ocean processes. Despite our progress, we still can't definitively distinguish between natural and human-caused changes, we don't fully understand the effects and roles of clouds and aerosols on climate, and we have limited ability to predict regional effects. More importantly, we have only begun to explore ways to mitigate and/or adapt to these effects. Ultimately, we need to be able to understand the factors that determine Earth's climate well enough to predict climate and climate impacts decades, or even centuries, in the future. We are developing the novel research tools, models, and integrated experi-

ments and computational science to find the answers.

**Target SC 3-2a:** Improve the precision of climate models by delivering a more realistic cloud submodel that reduces the uncertainty in calculations of the atmospheric energy budget by ten percent.

**Assessment and Commentary:** This target was met. A new cloud parameterization has been introduced into the Community Atmospheric Model with resulting improvements in cloud, radiation, and precipitation fields. The parameterization is currently being evaluated in the Atmospheric Radiation Measurement Parameterization Testbed through comparison with data and global data sets. Initial results from using the models indicate uncertainty has been reduced by approximately ten percent.

### **Advancing the Basic Science for Energy Independence:**

*Provide the scientific knowledge and tools to achieve energy independence, securing United States leadership and essential breakthroughs in basic energy sciences.*

The growth of our economy over the past half-century has derived in substantial part from steady improvements in our energy technologies. In each subsequent decade, we have produced more goods and services with a given amount of energy, and we have produced that energy more efficiently and with less environmental impact. Much of this progress has come from advances in the materials and chemical sciences such as new magnetic materials; high strength, lightweight alloys and composites; novel electronic materials; and new catalysts, with a host of energy technology applications.

We are now in the early stages of two remarkable explorations, observing and manipulating matter at the molecular scale and understanding the behavior of large assemblies of interacting components. Scientific discoveries in these new frontiers will accelerate our progress towards more energy efficient technologies and affordable, cleaner energy production methods needed for energy independence, economic growth, and a sustainable environment. They pose some of the most fascinating and far-reaching scientific challenges of our time:



*The Department's Nanoscale Science Research Centers.*

**Program Goal SC 4-2:** Enable United States leadership in nanoscale science, allowing the atom-by-atom design of materials and integrated systems of nanostructured components having new and improved properties for applications as diverse as high-efficiency solar cells and better catalysts for the production of fuels.

The main elements of the Department's nanoscale research program in Fiscal Year 2003 focused on the establishment of five Nanoscale Science Research Centers and the support for nanoscale research in targeted areas addressing forefront science and Departmental mission needs.

The Nanoscale Science Research Centers are a new way of doing business for the dispersed cottage industry of researchers currently working on the enormous set of problems that together define "nanoscale science." Each Nanoscale Science Research Center is connected to a major light or neutron source, allowing researchers to literally see, move, and create at the atomic level.

The ability to fabricate complex structures using chemical, biological, and other synthesis techniques; characterize them; assemble them; integrate them into devices; and do it all in one place will change the way materials research is done. This will allow the design of nanoparticles that can deliver medicines to specific

cellular sites, such as cancer cells, or the development of materials that can be used in aircraft and automobiles to self-repair stress cracks and other results of fatigue.

**Target SC 4-2a:** Begin construction of one Nanoscale Science Research Center, meeting the cost and schedule timetables within ten percent of the baselines given in the construction project data sheets.

**Assessment and Commentary:** This target was met. Critical Decision -3 was approved in February 2003 for the Oak Ridge National Laboratory, Nanoscale Science Research Center, allowing ground-breaking to occur in July 2003.

**Program Goal SC 7-4A:** Manage Basic Energy Sciences facility operations and construction to the highest standards of overall performance, using merit evaluation with independent peer review.

For more than half a century, the Department has envisioned, designed, constructed, and operated many of the premiere scientific research facilities in the world. Today, more than 8,000 researchers and their students from universities, other government agencies, private industry, and from abroad use these facilities each year — and this number is growing.



*The Advanced Photon Source at Argonne National Laboratory is a national synchrotron-radiation light source research facility funded by the Department. Using high-brilliance x-ray beams from the Advanced Photon Source, members of the international synchrotron-radiation research community conduct forefront basic and applied research in the fields of material science; biological science; physics; chemistry; environmental, geophysical, and planetary science; and innovative x-ray instrumentation.*

For example, the light sources built and operated by the Department now serve more than three times the total number of users they served in 1990. An indication of the ability of these research tools to build bridges between disciplines and open new vistas for research is seen in the dramatic increase — more than 20-fold in the last decade — of life science users at the light sources, once the sole domain of materials and physical science researchers.

**Target SC 7-4A2:** Maintain and operate the Basic Energy Science scientific user facilities so the unscheduled downtime on average is less than ten percent of the total scheduled operating time. Maintain the cost and schedule milestones within ten percent for upgrades and construction of scientific user facilities.

**Assessment and Commentary:** This target was met. Basic Energy Science user facilities have operated and performed according to the annual target.

### Delivering Computing for the Extremes of Science:

*Deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.*

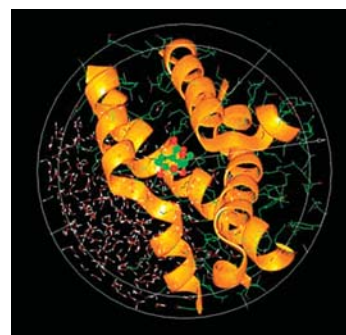
Computer-based simulation enables us to predict the behavior of complex systems that are beyond the reach of our most powerful experimental probes or our most sophisticated theories. Computational modeling has greatly advanced our understanding of fundamental processes of nature, such as fluid flow and turbulence or molecular structure and reactivity. Through modeling and simulation, we will be able to explore the interior of stars and learn how protein machines work inside living cells. We can design new catalysts and high-efficiency engines. Computational science is increasingly central to progress at the frontiers of almost every scientific discipline, and to our most challenging feats of engineering.

**Program Goal SC 5-2:** Create the Mathematical and Computing Systems Software and the High Performance Computing Facilities that enable

Scientific Simulation and Modeling Codes to take full advantage of the extraordinary capabilities of terascale computers, and the Collaboratory Software Infrastructure to enable geographically-separated scientists to effectively work together as a team as well as provide electronic access to both facilities and data.

Within the past two decades, scientific computing has become a cornerstone of all scientific research programs. Computation is particularly important for the solution of research problems that are insoluble by traditional theoretical and experimental approaches, hazardous to study in the laboratory, or time-consuming or expensive to solve by traditional means.

All of the research programs have identified major scientific challenges that can only be addressed through advances in scientific computing. The Office of Science Advanced Scientific Computing Research Program focuses on discovering, developing, and deploying advanced scientific computing and communications tools, and operation of the high-performance computing and network facilities that researchers need to analyze, model, simulate, and predict the behavior of complex natural and engineered systems.



*Model protein-substrate system used in a molecular dynamics simulation of yeast chorismate mutase.*

**Target SC 5-2a:** Begin installation of the next generation National Energy Research Scientific Computer-4, that will at least double the capability available to solve leading edge scientific problems.

**Assessment and Commentary:** This target was partially met. Procurement efforts for a next generation computer system could not produce a cost-effective independent new machine that could be installed in Fiscal Year 2003. However, the need to double capacity was addressed by doubling the size of the current National Energy Research Scientific Computer-3. The expanded National Energy Research Scientific Computer-3



was in full operation in March 2003, meeting performance expectations at a lower cost and shorter schedule than the planned National Energy Research Scientific Computer-4 approach.

**Target SC 5-2b:** Initiate at least five competitively selected interdisciplinary research teams to provide computational science and applied mathematics advances that will accelerate biological discovery in microbial systems or develop the next generation of computational tools required for nanoscale science based on peer review of submitted proposals.

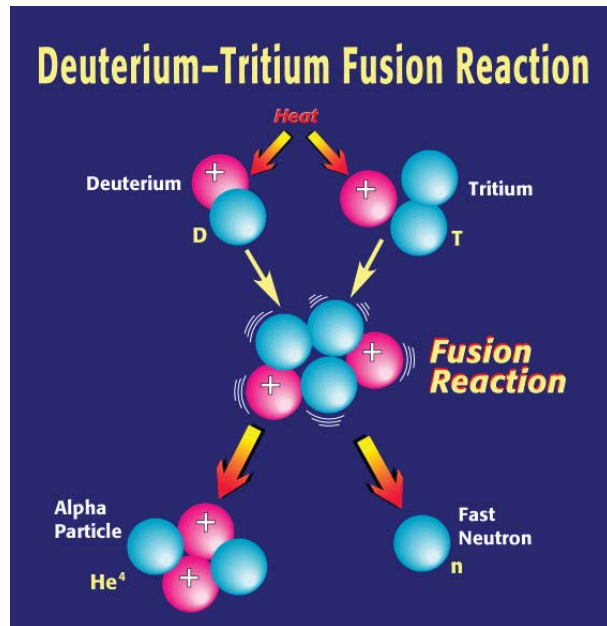
**Assessment and Commentary:** This target was met. Calls for proposals were prepared and issued and interdisciplinary research peer reviews completed as planned.

### Bringing the Power of a Star to Earth:

*Answer the key scientific questions and overcome enormous technical challenges to harness the power that fuels a star, realizing a landmark scientific achievement by bringing “fusion energy to the grid.”*

Fusion is the energy source that powers the sun and stars. Fusion energy science is a sub-field of plasma science that studies the fundamental processes taking place in plasmas where the temperature and density approach the conditions needed to allow the nuclei of low-mass elements such as hydrogen and helium isotopes to join together, or fuse, giving off tremendous amounts of energy. Power generated from fusion energy produces no troublesome emissions, is safe, and has few, if any, proliferation concerns. It creates no long-lived waste and runs on fuel readily available to all nations.

Making fusion energy a part of our national energy solution is among the most ambitious scientific and engineering challenges of our era. In Fiscal Year 2003, President Bush decided that the United States will join the negotiations for the construction and operation of a major international magnetic fusion research project. Known as the International Thermonuclear Experimental Reactor. The Project’s objective is to demonstrate the scientific and technical feasibility of fusion energy for peaceful purposes.



**Fusion Reaction:** Fusion, the energy source of the sun and other stars, is a reaction process that converts matter into energy. Fusion occurs in plasmas when two nuclei of hydrogen, such as deuterium or tritium are combined (fused) together under enormous temperature and pressure to form a single nucleus of helium. During the fusion process, some of the matter involved in the reaction is converted directly into a much larger amount of energy. For example, the amount of deuterium in one gallon of sea water would yield the energy equivalent of 300 gallons of gasoline.

**Program Goal SC 6-1:** Develop the basis for a reliable capability to predict the behavior of magnetically-confined plasma, and use the advances in the Tokamak concept to enable the start of the burning plasma physics phase of the United States’ fusion sciences program. Several inventive configurations of magnetic fusion have been proposed to confine the plasma as it is heated to the conditions necessary for fusion. However, progress leading to practical fusion energy is paced by scientific understanding of magnetically-confined hot plasmas, a turbulent mix of charged particles subject to magnetic and electric fields, and by advances in certain critical technologies.

**Target SC 6-1c:** Produce high temperature plasmas with five megawatts of Ion Cyclotron Radio Frequency power for pulse lengths of 0.5 seconds in the Alcator C-Mod. Assess the stability and confinement properties of these plasmas, which would have collisionalities in the same range as that expected for the burning plasma regime.



*Magnetic fusion relies on magnetic forces to confine the charged particles of the hot plasma fuel for sustained periods of fusion energy production.*

**Assessment and Commentary:** This target was met. Five megawatts of Ion Cyclotron Radio Frequency power, with a 0.5 second pulse length, was produced and assessed. Results were obtained from these experiments and analyzed. A report was prepared and submitted to the Department in September 2003.