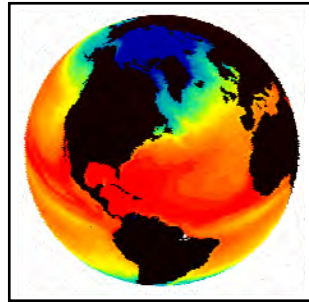
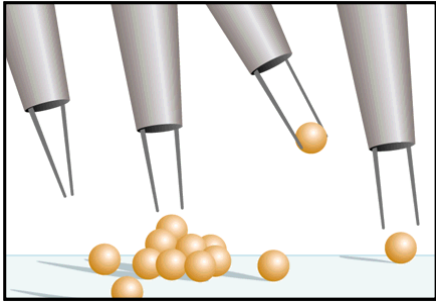
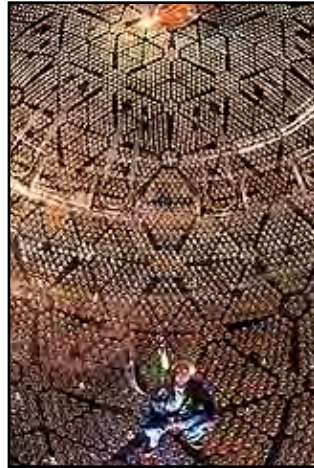
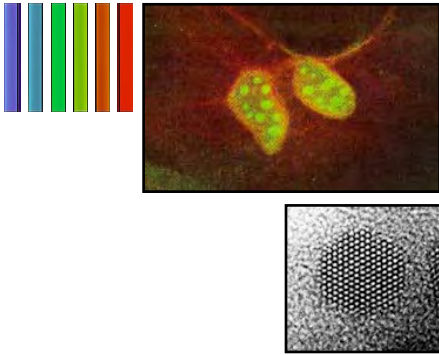




Advanced Scientific Computing Advisory Committee



The FY 2002 Office of Science Budget Request



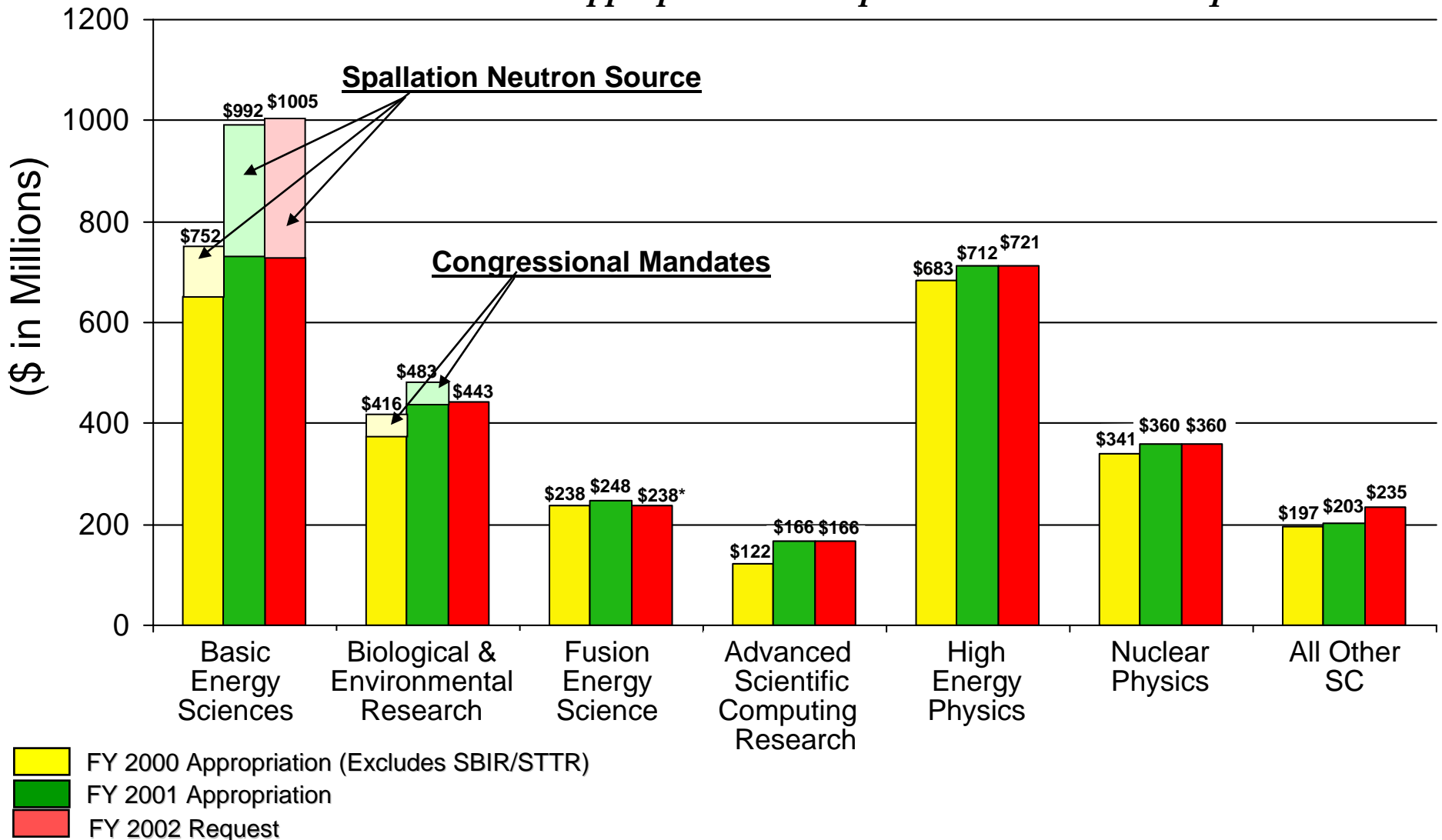
Science for America's Future

**Dr. James Decker
Acting Director,
Office of Science**

May 2, 2002

DOE Office of Science Budget

FY 2000 and FY 2001 Appropriation Comparable to FY 2002 Request



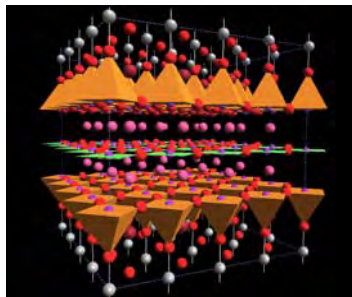
* An additional \$10M will be transferred to Fusion Energy Sciences through a budget amendment to be transmitted to Congress shortly. The source for this \$10 M is: High Energy Physics (\$5.0M), Advanced Scientific Computing Research (\$2.7M), Energy Research Analysis (\$0.3M), and Science Program Direction (\$2.0M)

DOE Office of Science FY2002 Budget Highlights

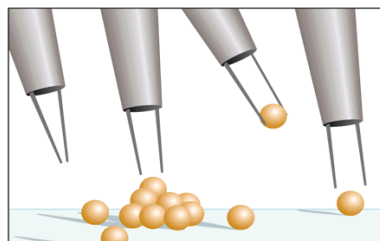
(FY2002 Request)



- Spallation Neutron Source (\$291M)



- Scientific Discovery through Advanced Computing (\$176M)



- Nanoscale Science, Engineering, & Technology (\$87M)

- Genomes to Life (\$20M)



- The High Energy Physics Frontier (\$721M)



- Fusion Energy Sciences (\$248M)

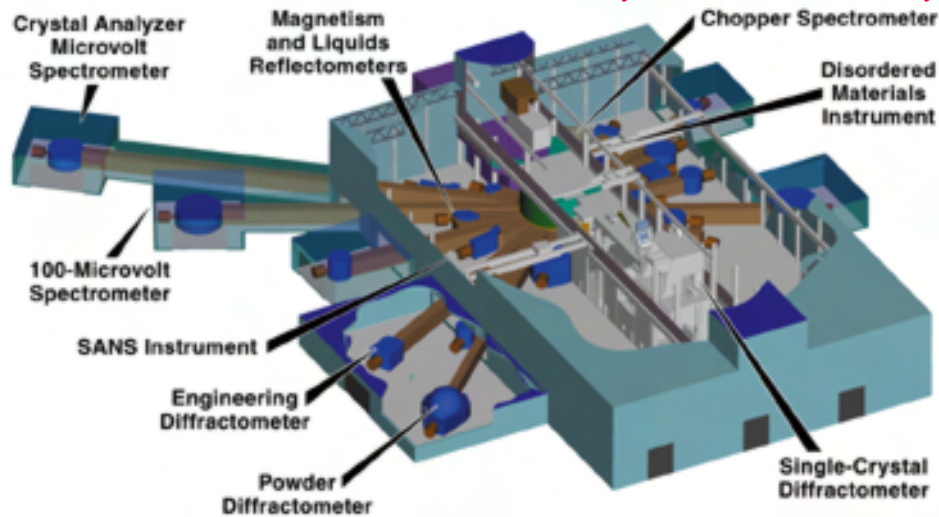
- Science Education (\$5.5M)

The Spallation Neutron Source (SNS)

Under Construction on Chestnut Ridge at ORNL

Schematic instrument suite for the SNS.

Final instrumentation will be determined by the user community



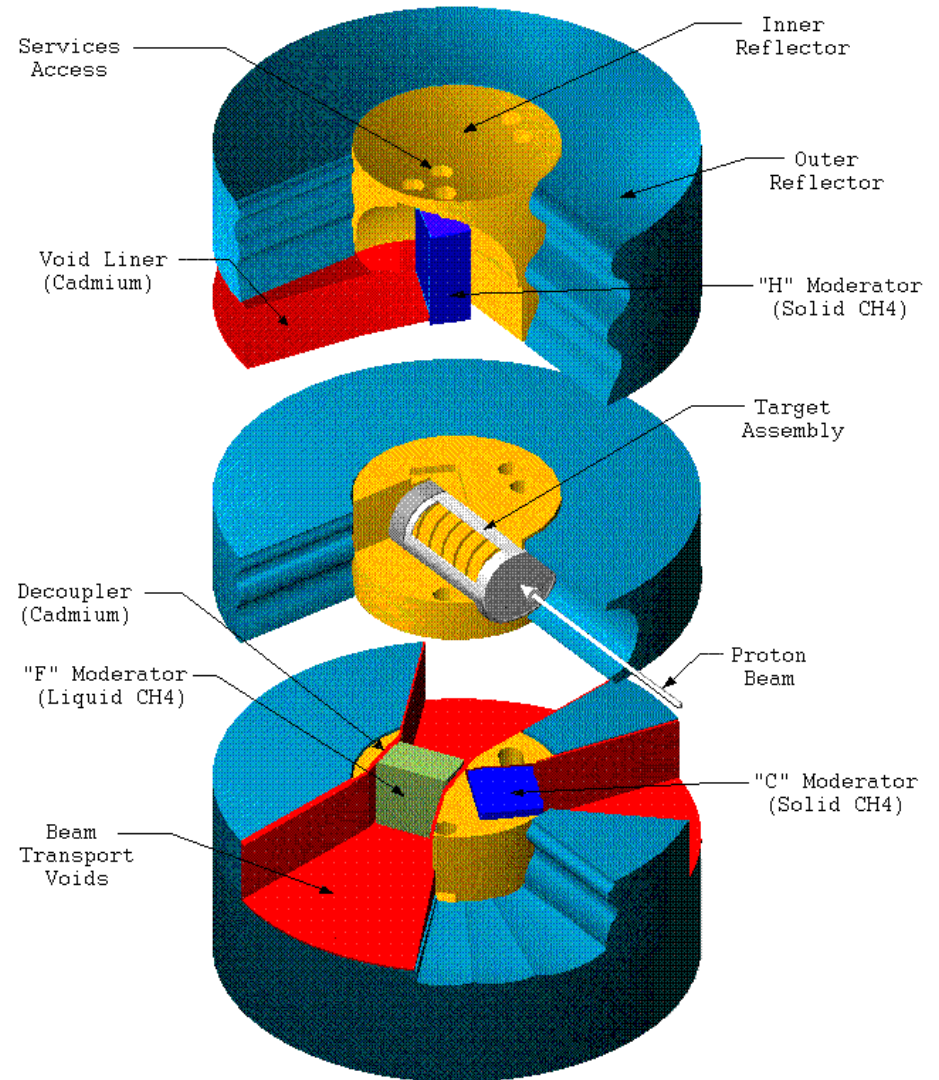
- World's premier neutron scattering facility for basic and applied research in physical, materials, polymer, chemical, and biological sciences. Expected to host more than 2000 researcher a year.
- FY 2001 activities – begin: Title II design, site preparation, subsystem fabrication, conventional facility construction
- FY 2002 requirement - \$291M
- FY 2002 activities – continue: conventional facility construction, design and procurement of accelerator and global control systems. Begin installation of Linac components, Ion source and low energy beam equipment, target and instrument systems design
- Project on track to meet Level 0 (Secretarial) baseline goals.
 - Total Project Cost - \$1,411.7 M
 - ≥ 1 MW proton beam power on target
 - Project completion – June 2006



Artist's Conception of the Finished Facility Overlaid on the October 2000 Aerial View

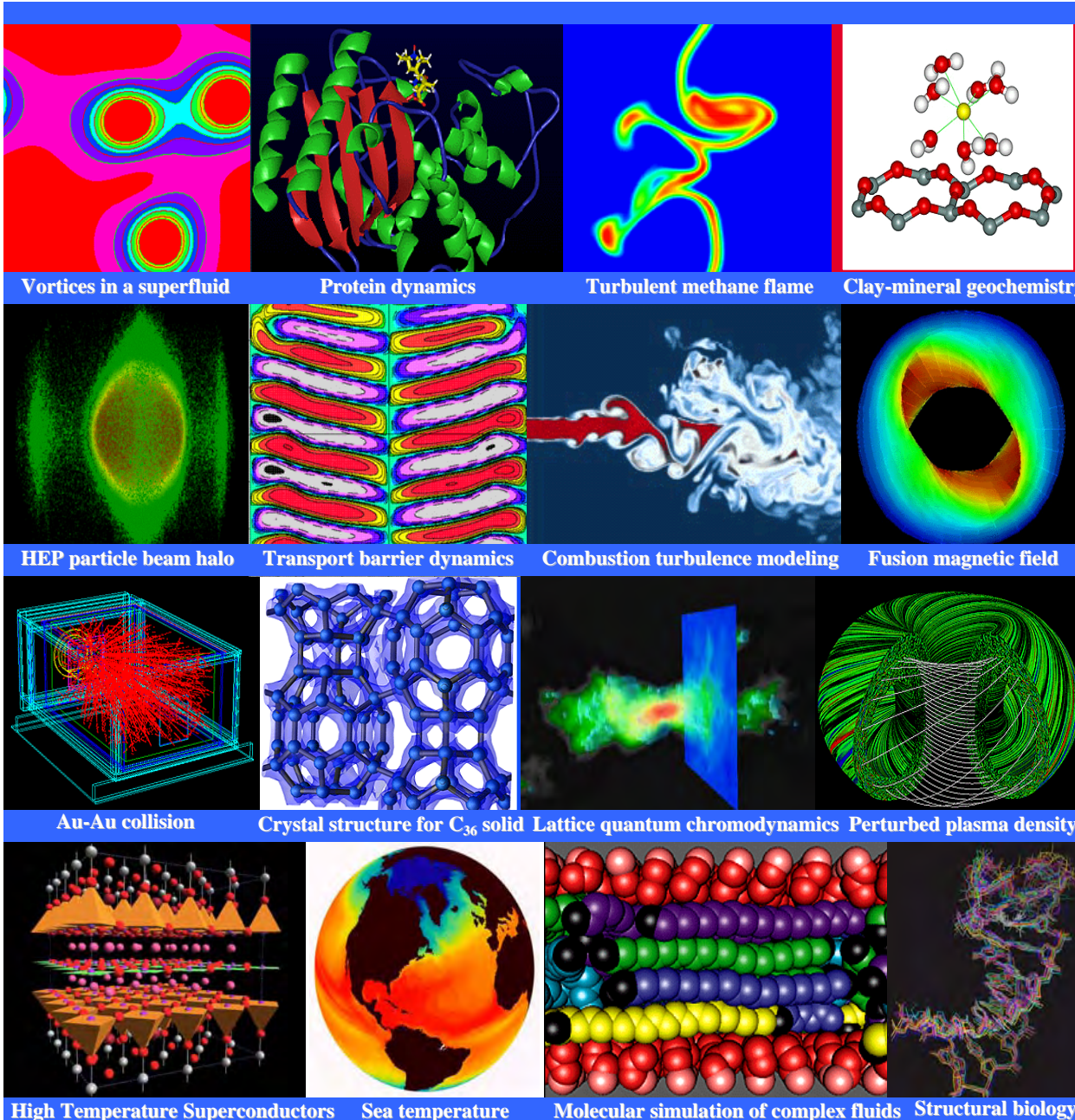
Expanded Operations at Key Facilities in FY02

- Intense Pulse Neutron Source (IPNS)
 - Instrumentation upgrades and increased operating time
- Environmental Molecular Sciences Laboratory (EMSL)
 - Terascale computing capabilities
- Fermilab
 - Increased operating time and detector enhancements
- SLAC
 - Increased operating time
- National Energy Research Scientific Computing (NERSC)
 - Terascale computing capabilities

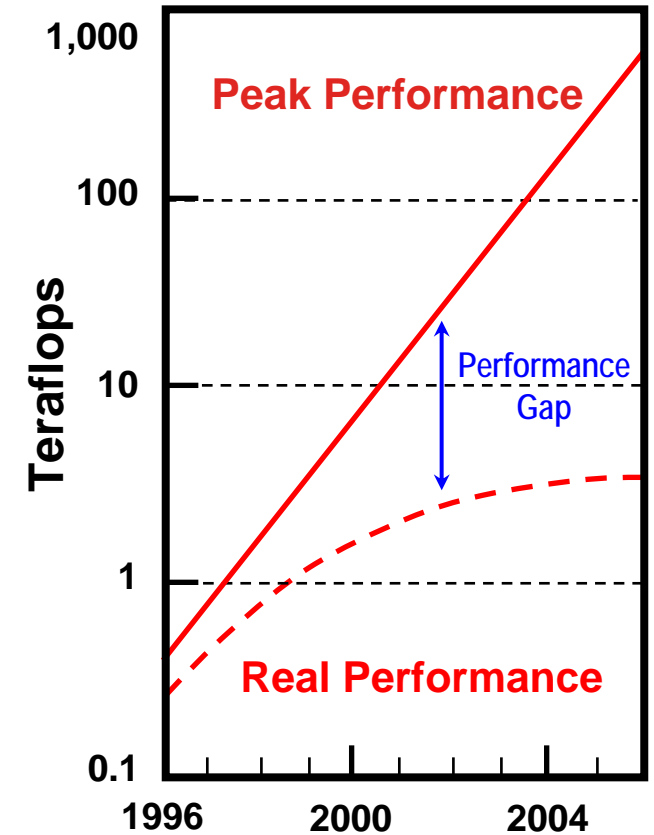


The IPNS target-reflector-moderator assembly

Scientific Discovery Through Advanced Computing



Peak Performance is skyrocketing



But efficiency declining

From 40-50% on the vector super-computers of 1990s to as little as 5-10% on parallel supercomputers of today

Scientific Discovery Through Advanced Computing

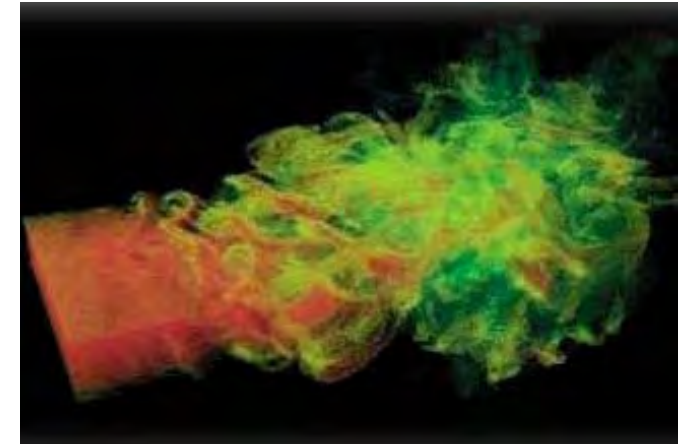
Using Supercomputers To Revolutionize Science

- **New Software Infrastructure**

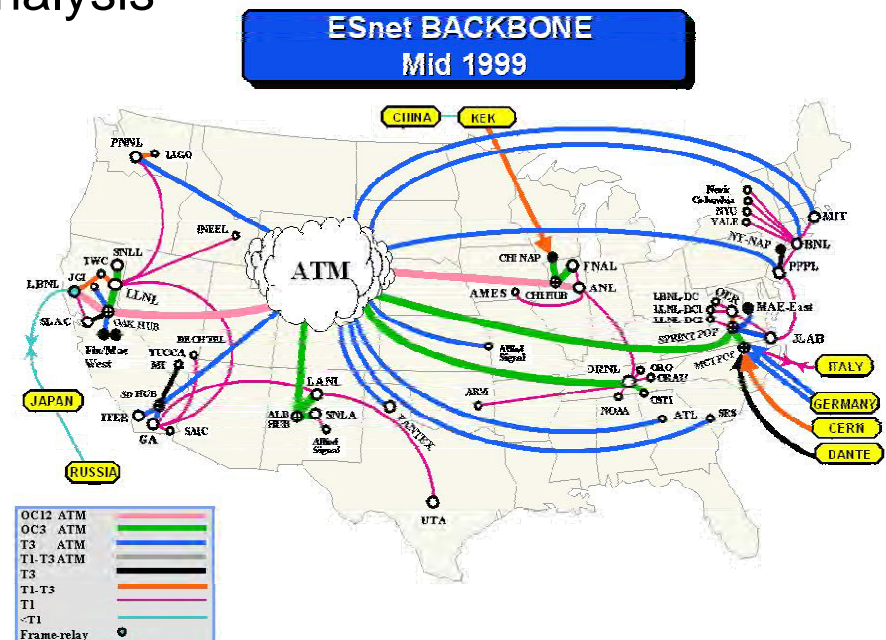
- Operating systems and software tools to optimize total system
 - Processors – Memory - Communications channels - Disk drives
- Algorithms that can use thousands of processors
- Petabytes data set management & analysis software
- Advanced collaboratory software

- **Modeling And Simulation**

- Basic theory development
- Scientific code development by interdisciplinary teams
- Code validation through experiment



Combustion Models & Simulations

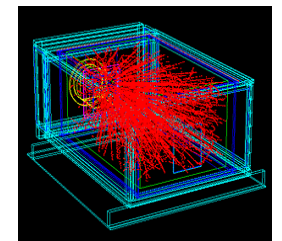
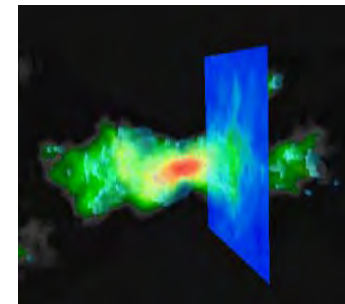
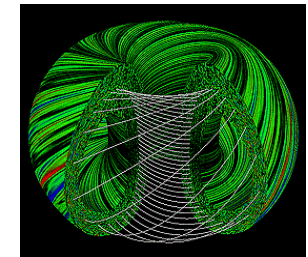
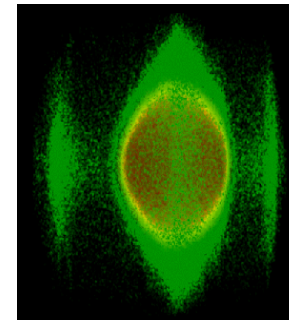
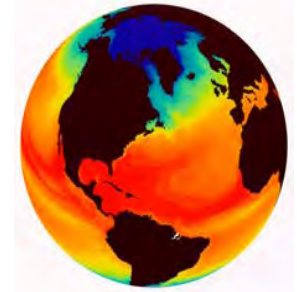
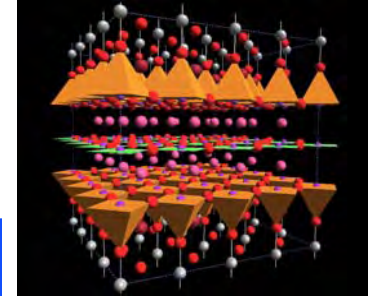
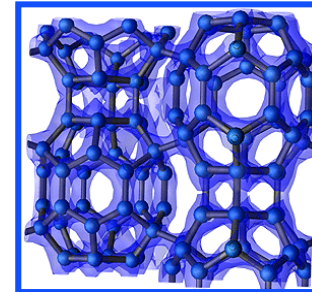


FY 2001 Scientific Discovery Through Advanced Computing Activities

- Solicitations were made to universities and laboratories for approximately \$53 million for new FY 2001 funding focusing on R&D to support DOE-specific activities in three areas of Advanced Computing:
 - high performance middleware services that provide ease of collaboration for distributed teams;
 - innovative, high performance network research that is focused on improving the end-to-end performance for data intensive scientific applications; and
 - laboratories to test and validate the enabling technologies for discipline-specific applications.
- Over 160 preproposals were received from labs, universities and lab-university collaborations. An impressive response from the scientific community. Formal Applications due March 15, 2001.
 - 50% were mailed Encouragement letters
 - 50% were mailed Discouragement letters

FY 2001-2002 Scientific Discovery Through Advanced Computing Activities

- Approximately \$53M new FY01 funding:
 - National Collaboratories & High Performance Networks
 - Integrated Software Infrastructure Centers
 - Scientific Applications
 - *Energetics & dynamics of chemical reactions*
 - *Chemistry & fluid dynamics interaction*
 - *Climate at regional & global scales for decades to centuries, including uncertainty*
 - *Microscopic turbulence & macroscopic stability in magnetically confined plasmas*
 - *Basic plasma science processes*
 - *Beam dynamics and electromagnetic fields in inertial fusion accelerators*
 - *Beam dynamics and electromagnetic fields in particle accelerators*
 - *Large scale simulations of QCD (fundamental theory governing strong interactions)*
 - *Supernovae explosions*
 - *Collaboratory pilot projects for large experiments*

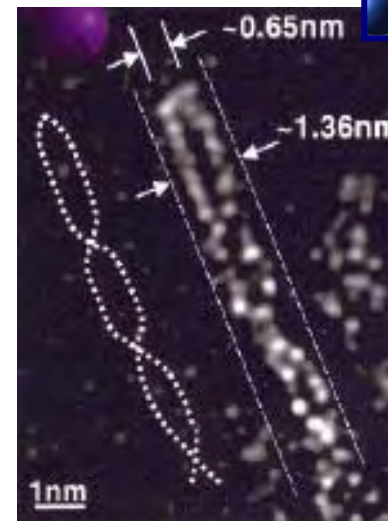
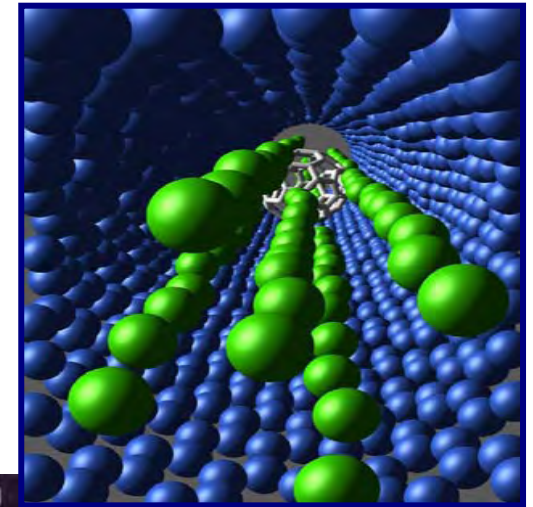


Nanoscale Science, Engineering, & Technology

Building Structures One Atom at a Time

- Tailor materials at the nanoscale for desired structure/function properties
 - *Materials with enhanced physical, mechanical, optical, electrical, tribological, or catalytic properties*
 - *Materials with the ability to self assemble, self repair, sense and respond to the environment*
- Combines expertise in materials sciences, chemistry, physics, biology, engineering, and computation
- Expected are technological developments to rival the impact of the transistor

Fluid flow in a nanotube

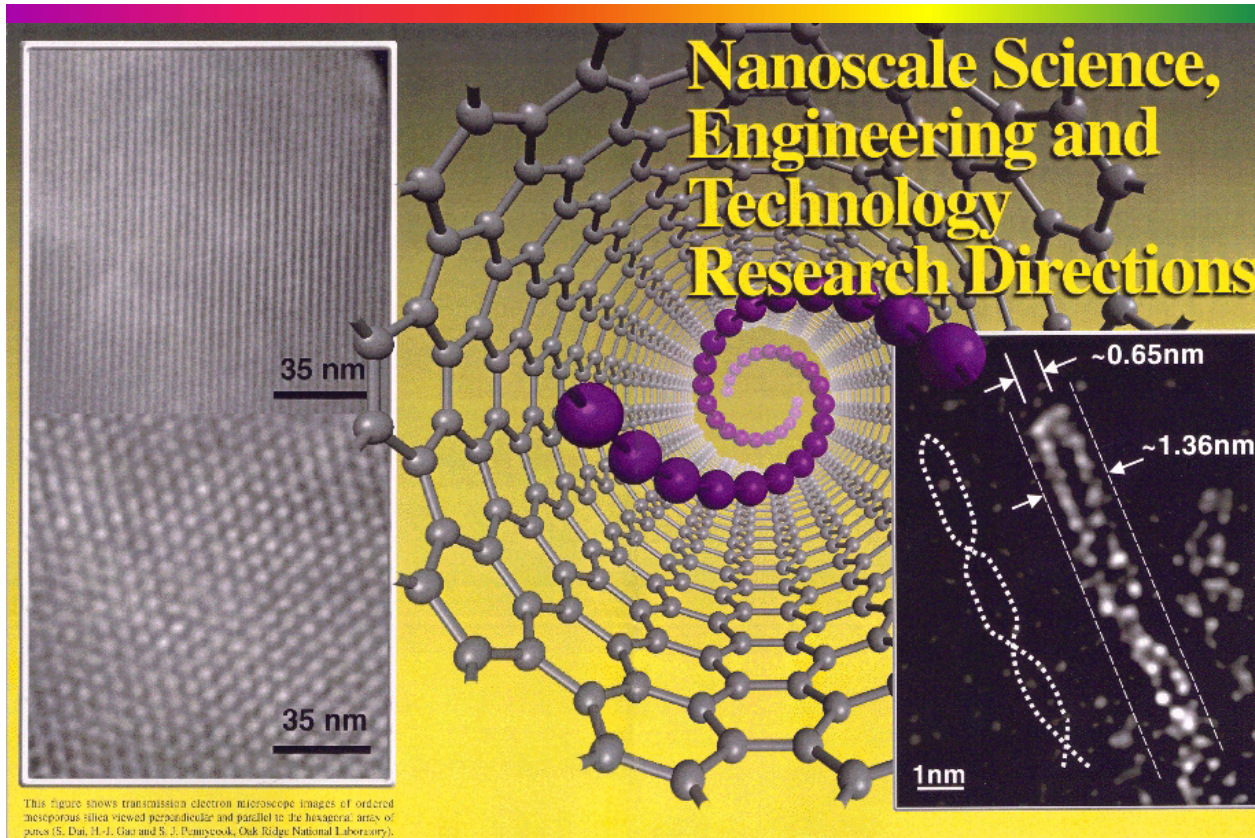


A Z-contrast transmission electron microscope image of iodine atoms intercalated inside a single-wall carbon nanotube in the form of a double helix (ORNL, U. Kentucky and Vanderbilt U.).

FY 2001 Nanoscale Science Activities

- Solicitations were made to universities and labs for approximately \$30 million new FY 2001 funding.
 - 745 preproposals were received from universities! An enormous response from the scientific community. (313 Encouragement letters mailed)
 - 497 formal applications were received March 14.
- 46 proposals were received from laboratories. (The labs were limited to 4 responses per lab for large group activities.)
- Planning for Nanoscale Science Research Centers (NSRC) was initiated.
- About \$3M was used to support increased facility operations for Nanoscale research.

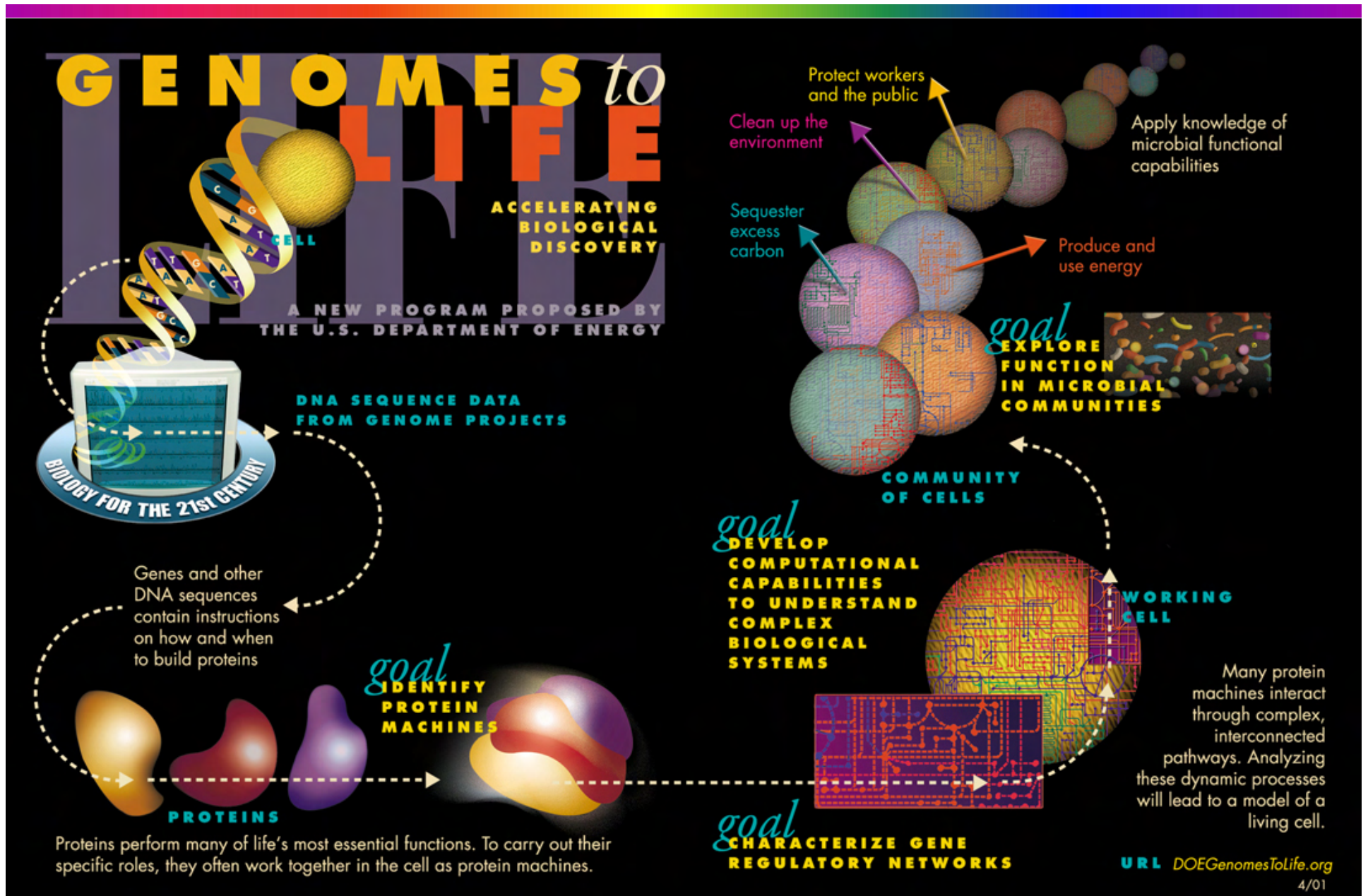
FY 2001 Proposed Nanoscale Science Research Areas



- Materials Chemistry
- Engineering Research
- Separations and Analysis
- Geosciences
- Physical Behavior of Materials
- Synthesis and Processing

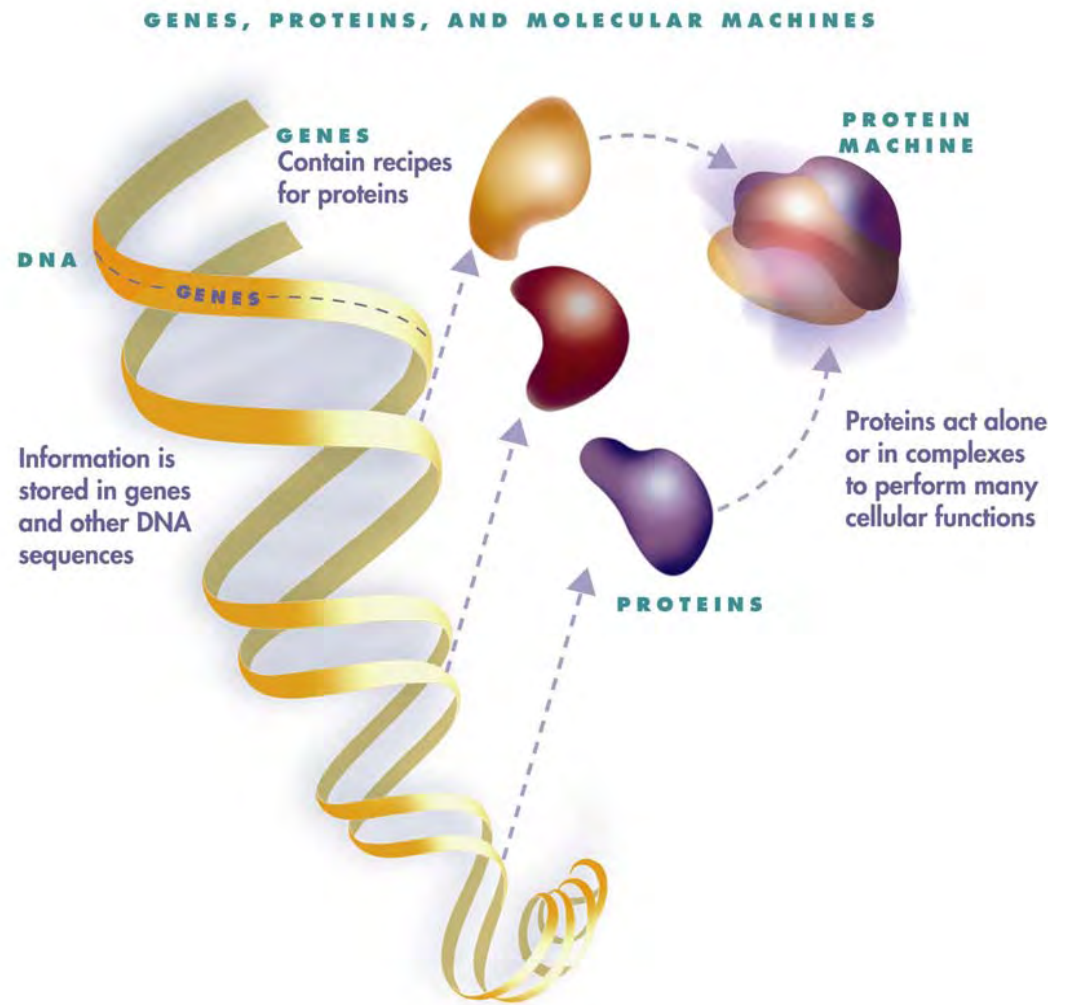
- Structure and Composition of Materials
- Mechanical Behavior and Radiation Effects
- Experimental and Theoretical Condensed Matter Physics
- Chemical Energy and Chemical Engineering
- Catalysis and Chemical Transformations

Beyond Genome Sequencing



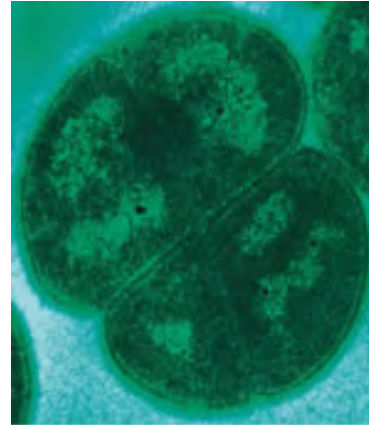
Goals of Genomes to Life Programs

- Identify and characterize the molecular machines of life—the multi-protein complexes that execute cellular functions and govern cell form.
- Characterize gene regulatory networks.
- Characterize the functional repertoire of complex microbial communities in their natural environments at the molecular level.
- Develop the computational methods and capabilities to advance understanding of complex biological systems and predict behavior.



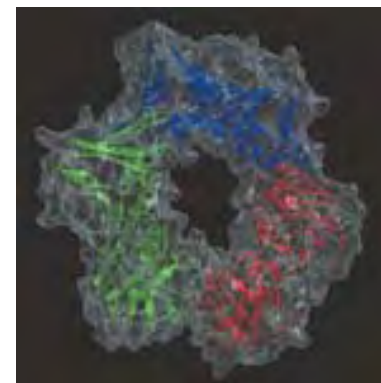
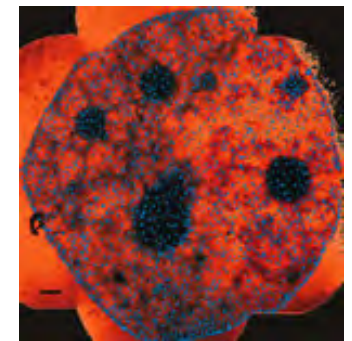
Biological Solutions for DOE Missions

- Human Susceptibility
- Bioremediation
- Chemical and Biological National Security
- Renewable and Alternative Energy Sources
- Carbon Cycle and Sequestration



D Radiodurans - Knowledge about the metabolic & regulatory pathways of microbes will help to begin understanding and using their remarkable capabilities, especially those related to environmental remediation, biogeochemical cycles, climate changes, and energy production.

This image of a human mammary cell was produced using soft X-ray microscopy at LBNL. The blue dots label proteins of the nuclear pore complex, through which molecules enter and exit the nucleus.



The role of the Rad checkpoint complex was inferred from the 3-D structure predicted by comparative modeling at Lawrence Livermore National Laboratory. The Rad complex delays cell division to allow time for DNA repair to take place.

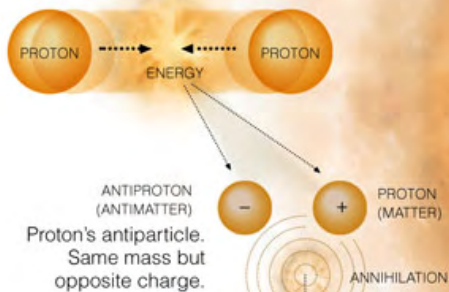
An Exciting Time for Physics

Pursuing Asymmetry in the Universe

A perfectly symmetrical universe would be empty — equal amounts of matter and antimatter would annihilate each other. So far, though, it looks like there is an overabundance of matter. Physicists are searching for slight differences in particle behavior to explain the asymmetry.

1 MATTER AND ANTIMATTER

Scientists can generate a burst of energy by smashing particles into each other. Both matter and antimatter can emerge from such collisions.



A particle and its antiparticle annihilate when they meet. That is, they disappear, and the

November 21, 2000

Particle Physics Braces for the Next Big Thing

By JAMES GLANZ

GENEVA — Gerard Bachy, an engineer, stands 250 feet underground in an immense, bottle-shaped cavern the world might regard as a lantern. Thousands in effect, to rub this mysterious subatomic Higgs boson that they say is the source of the reason matter has

If they are granted, scientists may find by more speculative dimensions beyond



Tuesday January 16, 2001

YAHOO! NEWS

Highest Density of Matter Created



STONY BROOK, N.Y. (AP) - Scientists say they used a particle accelerator to smash the nuclei of gold atoms together to make the highest density of matter ever created in an experiment.

The accelerator, the Relativistic Heavy Ion Collider, smashed the nuclei together at nearly the speed of light, Brookhaven National Laboratory scientists said at a conference Monday. Physicists who studied the debris streaming from the collisions concluded that densities more than 20 times higher than those within the nuclei of ordinary matter had been produced.

November 9, 2000

Race to Find Basis of Mass Still on as Lab Retires Device

By JAMES GLANZ

GENEVA, Nov. 8 — The director of the leading European particle physics laboratory has decided to shut down a particle accelerator here just as scientists using it believed they were on the verge of capturing one of the most glittering prizes in physics: the discovery of the particle that theorists believe is the origin of all mass in the



Dr. Morse presenting results of Brookhaven's experiment.

February 13, 2001

The New York Times

Particle Physics Gets Modern-Day 'Eureka!'

By JAMES GLANZ

Archimedes shouted "Eureka!" when he discovered how to tell what an apparently gold crown was really made of without tearing it apart. Last week, particle physicists at Brookhaven National Laboratory said they had found hints of a new form of matter using a remarkably similar trick.

Instead of dunking a crown and measuring how much water it displaced, as Archimedes did, the physicists dipped

July 21, 2000

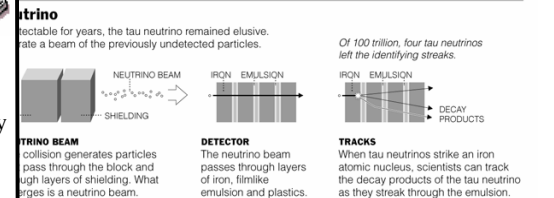
The New York Times

Scientists Detect Elusive Building Block of Matter

By JAMES GLANZ

What many physicists consider to be one of the last pieces of the theoretical puzzle that explains the structure of matter has been detected at the Fermi National Accelerator Laboratory near Chicago.

An international team of scientists will announce today that they have detected the tau neutrino, considered to be the most elusive member of nature's most ghostly family of particles, the neutrinos.



June 22, 1999

The New York Times

Physicists Zero In on Ghostly Neutrinos

By MALCOLM W. BROWNE

Scientists operating huge underground detectors in Japan and Canada are racing to obtain independent proofs that the elusive neutrino, a ghostly particle whose vast family may constitute a large part of the mass of the universe, changes form as it flies through matter or space.

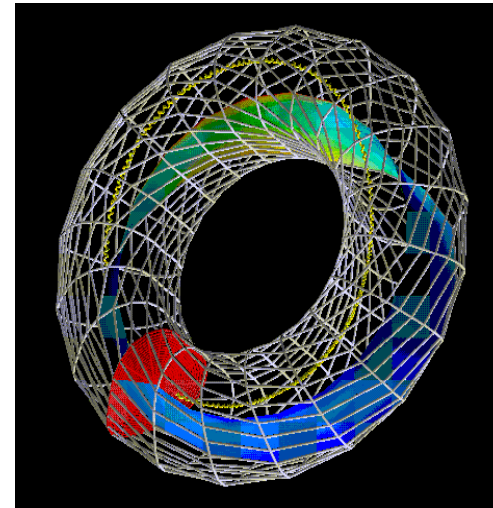
A race to prove that a pervasive particle changes its form.

At least some neutrinos are now believed to have some mass, and physicists would love to learn how much, a goal that may be reached by studying the changes in form a traveling neutrino undergoes.

At issue is the effect of neutrinos, which pervade every cubic inch of

Science-Based Fusion Energy Research

- Improve and extend our understanding of how to confine a plasma, hotter than the sun, in toroidal magnetic fields.
- Understand the fundamental processes of plasmas and predict their complex behavior through the development of integrated computer models.
- Develop heavy ion accelerators and compare to beam simulation codes for possible Inertial Fusion Energy drivers.
- In partnership with NSF, support basic plasma science and engineering.
- Support a Junior Faculty in Plasma Science development program.
- Successfully and safely complete the decontamination and decommissioning of the Tokamak Fusion Test Reactor.

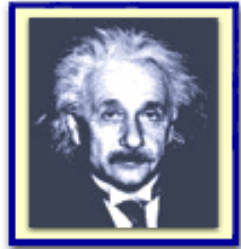


This picture demonstrates particle trajectories and electrostatic potentials from a 3D implicit tokamak plasma simulation employing adaptive mesh techniques.



Removal of the TFTR Umbrella Structure

Science Education



- Signed an agreement with NSF in 2000 to jointly fund and expand Science Education at the DOE National Laboratories
- \$5.5 Million core program in Science Program Direction
 - *Undergraduate Research Fellowships Program*
 - *Community College Program*
 - *National Science Bowl*
 - *Albert Einstein Distinguished Educator Fellowship*





Backup

Office of Science Results & Recognition

**SCIENCE
MAGAZINE**



Breakthrough of the Year: *Genome Sequencing*

The editors at the international journal, Science, have compiled their list of the Top 10 scientific developments for the year 2000, placing genome sequencing first on the list.

Science's Top 10 research advances, chosen for their profound implications for society and the advancement of science, appear in the journal's 22 December 2000 issue.

These advances will bring with them a host of ethical questions that we have only begun to address. Yet, genome sequencing's potential for advancing human health and our understanding of life has made it irresistible.

Science also salutes nine other scientific achievements of 2000.

Except for the first runner up, the others are in no particular order.

RNA Runs the ribosome: Last year witnessed the

unveiling of the first molecular maps of the ribosome, the essential protein factory. In 2000, higher-resolution maps of the ribosome revealed startling details about its structure and support for an "RNA world" as the model for the origin of Earth. Although the ribosome consists of both ribosomal RNA (rRNA) and proteins, researchers found that the "active site" of the ribosome--the site of the chemical reaction

The New York Times

June 8, 1999

Systems Designed to Hold a Homemade Sun

Scientists have developed a variety of devices and systems in which they hope to be able to compress hydrogen to the densities and temperatures needed to sustain thermonuclear fusion reactions. These are among them.



January 19, 2001

The Washington Post

Celera and National Labs to Collaborate

By Justin Gillis

The Sandia National Laboratories and Celera Genomics Corp. will announce a collaboration this morning to speed computer analyses of biological data, perhaps solving in hours problems that now take months of computer time.

Light Beams May Find Breast Cancer

By MICHELLE LOCKE, Associated Press Writer

LIVERMORE, Calif. (AP) - Lawrence Livermore nuclear scientists

July 21, 2000

The New York Times

Scientists Detect Elusive Building Block of Matter

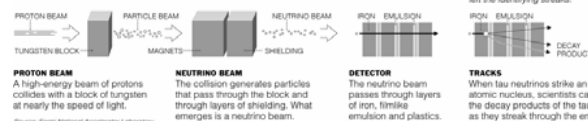
By JAMES GLANZ

What many physicists consider to be one of the last pieces of a theoretical puzzle that explains the structure of matter has been detected at the Fermi National Accelerator Laboratory near Batavia, Ill.

HOW THEY DID IT

The Search for the Tau Neutrino

While two types of neutrinos have been detectable for years, the tau neutrino remained elusive. Scientists used a beam of protons to generate a beam of the previously undetected particles.



Source: Fermi National Accelerator Laboratory

Jan. 19, 2001

REUTERS

Study Unlocks Brain Mystery of Ritalin

By Merritt McKinney

NEW YORK (Reuters Health) - Doctors have been prescribing Ritalin for years to treat attention-deficit/hyperactivity disorder (ADHD) in children, but exactly how the stimulant helps young people calm down and pay attention has been unclear.

Now, researchers at the Brookhaven National Laboratory in Upton and the State University of New York at Stony Brook report that the medication appears to work by increasing levels of the brain chemical dopamine. And

Tuesday January 16, 2001

YAHOO! NEWS

Highest Density of Matter Created



STONY BROOK, N.Y. (AP) - Scientists say they used a particle accelerator to smash the nuclei of gold atoms together to make the highest density of matter ever created in an experiment.

The accelerator, the Relativistic Heavy Ion Collider, smashed the nuclei together at nearly the speed of light, Brookhaven National Laboratory scientists said at a

conference Monday. Physicists who studied the debris streaming from the collision at densities more than 20 times higher than ordinary matter had been produced. The compressed matter topped 1 trillion degrees.

AP Associated Press

January 21, 2001

The New York Times

June 27, 2000

Genetic Code of Human Life Is Cracked by Scientists

By NICHOLAS WADE

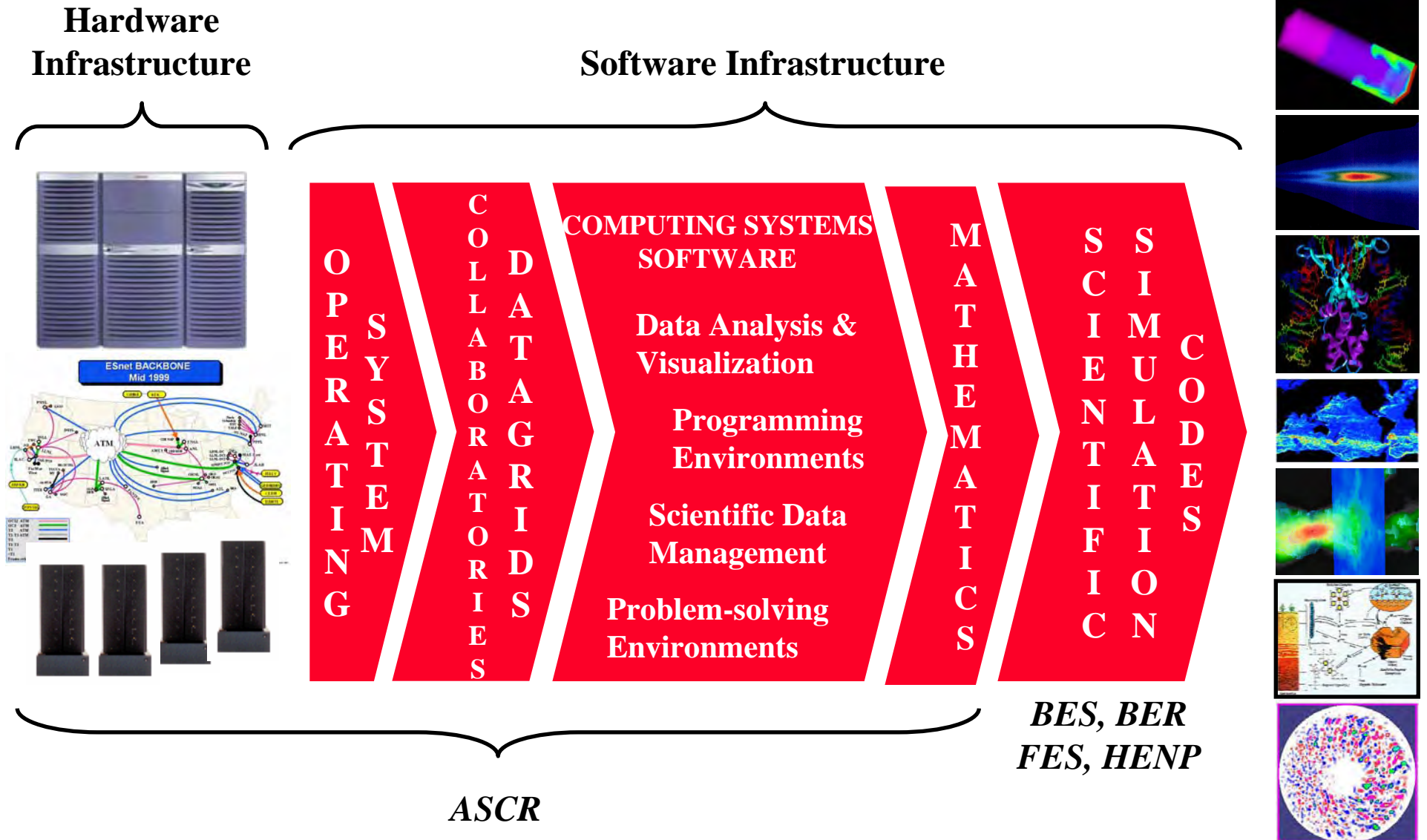


Dr. Francis Collins and J. Craig Venter joined President Bill Clinton at the White House on Monday to announce the completion of the first draft of the human genome.

WASHINGTON, June 26 -- In an achievement that represents a pinnacle of human self-knowledge, two rival groups of scientists said today that

Scientific Computing Infrastructure

What we are Doing to Bridge the Performance Gap



Scientific Computing Infrastructure

What we are Doing to Bridge the Performance Gap

