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

- 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
  - ≥1MW proton beam power on target
  - Project completion – June 2006
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
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
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
- collaboratories 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
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.

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 that scientists around the world might regard as a kind of magic lantern. Thousands of those scientists hope, in effect, to rub this lantern and conjure a mysterious subatomic particle called the Higgs boson that their most trusted theories say is the source of all mass in the universe, the reason matter has weight.

If they are granted a few more wishes, those scientists may find strange things predicted by more speculative theories, like new dimensions, beyond the usual four, hidden in the fabric of space, and swarms of other unknown particles with odd properties — discoveries that would remake humanity's view of the cosmos.

February 13, 2001

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...
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.
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
**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 has 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 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 ribonucleic acid (rRNA) and proteins, researchers found that the “active site” on the large unit of the ribosome—the site of the chemical reaction that changes genetic information into the beginnings of a protein—contains only rRNA. This suggests that the ribosome is actually a ribozyme, an RNA molecule that can catalyze its chemical reactions. RNA’s starring role in the ribosome may support the idea that life on Earth is the product of an “RNA world” as the model for the origin of life.

**Light Beams May Find Breast Cancer**

By MICHELLE LOCKE, Associated Press Writer

LIVERMORE, Calif. (AP) - Lawrence Livermore nuclear military laboratory scientists are working on a new weapon in the fight against breast cancer, a probe that uses Light Beams to probe breast tissue.

**Systems Designed to Hold a Homemade Sun**

By JAMES GLANZ

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.

**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.
Scientific Computing Infrastructure

What we are Doing to Bridge the Performance Gap

Hardware Infrastructure

- Operating System
- Collaboratories
- Data Grids

Software Infrastructure

- Computing Systems Software
  - Data Analysis & Visualization
  - Programming Environments
  - Scientific Data Management
  - Problem-solving Environments

Mathematics

Scientific Simulation Codes

BES, BER
FES, HENP

ASCR
Scientific Computing Infrastructure
What we are Doing to Bridge the Performance Gap

Hardware Infrastructure
- ASPR
- BES, BER, FES, HEP, NP

Software Infrastructure
- Fundamental Research
- R&D for Applications
- Testbeds
- Scientific Simulation Codes

- Applied Mathematics
- Computer Science
- Advanced Computing Software Tools
- Scientific Application Pilots
- Integrated Software Infrastructure Centers
- Groups of mathematicians, computer scientists, application scientists, and software engineers

Facilities
- National Energy Research Scientific Computing Center (NERSC)
- Advanced Computing Research Facilities
- Energy Sciences Network (ESnet)

- Networking
- Collaborative Tools
- Collaboratory Pilots
- Facility Access
- Teams of Researchers

- Applications
  - Materials
  - Chemical
  - Combustion
  - Accelerator
  - HEP
  - Nuclear
  - Fusion
  - Global Climate
  - ...

Enhanced

ESnet BACKBONE
Mid 1998