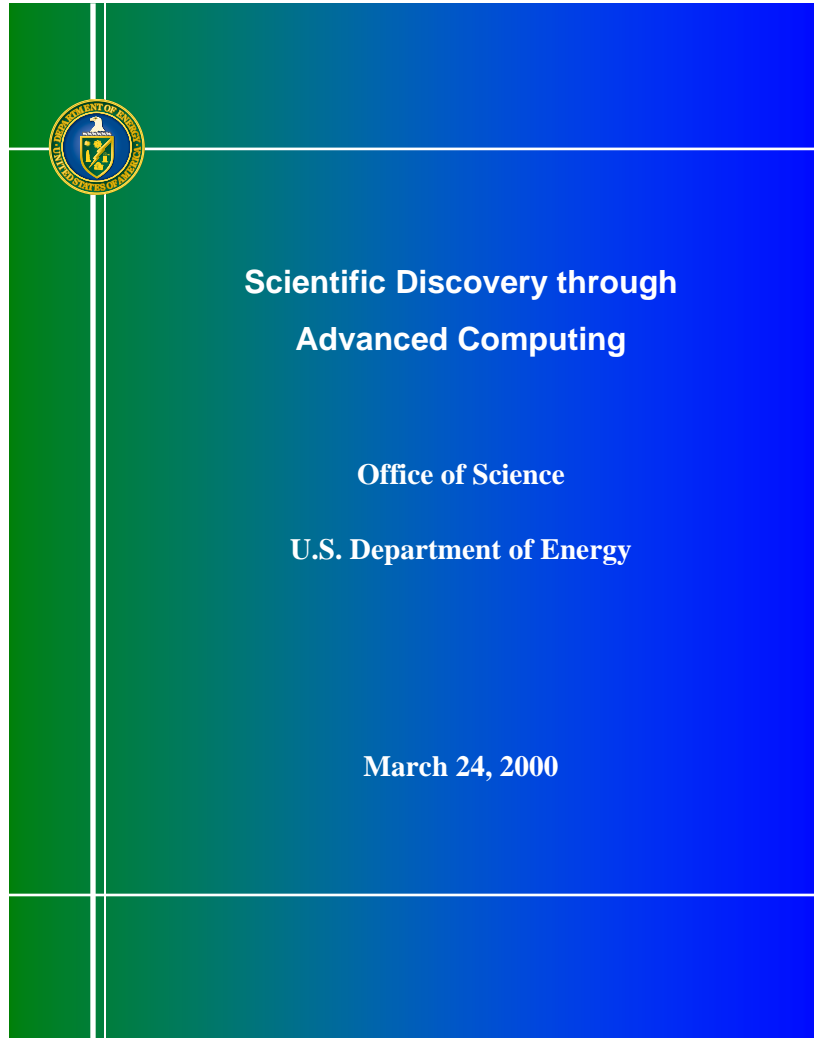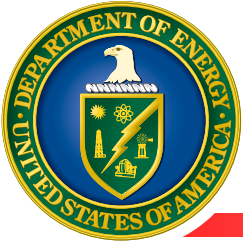# Report on "Scientific Discovery through Advanced Computing" to the Advanced Scientific Computing Advisory Committee

Stephen Eckstrand

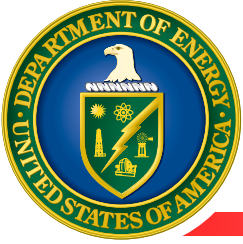**Office of Science**

U.S. Department of Energy

Office of Science Computing Plan

Scientific Discovery through

Advanced Computing

Office of Science

U.S. Department of Energy

March 24, 2000

On March 30, 2000 the Office of Science submitted a plan for scientific computing to the Energy & Water Development Subcommittees of the Appropriations Committees of the U.S. Congress.

The plan, titled "Scientific Discovery through Advanced Computing," outlined a five-year program to develop the *Scientific Computing Software* and *Hardware Infrastructure* needed to use terascale computers to advance its research programs in basic energy sciences, biological and environment research, fusion energy sciences, and high energy and nuclear physics.
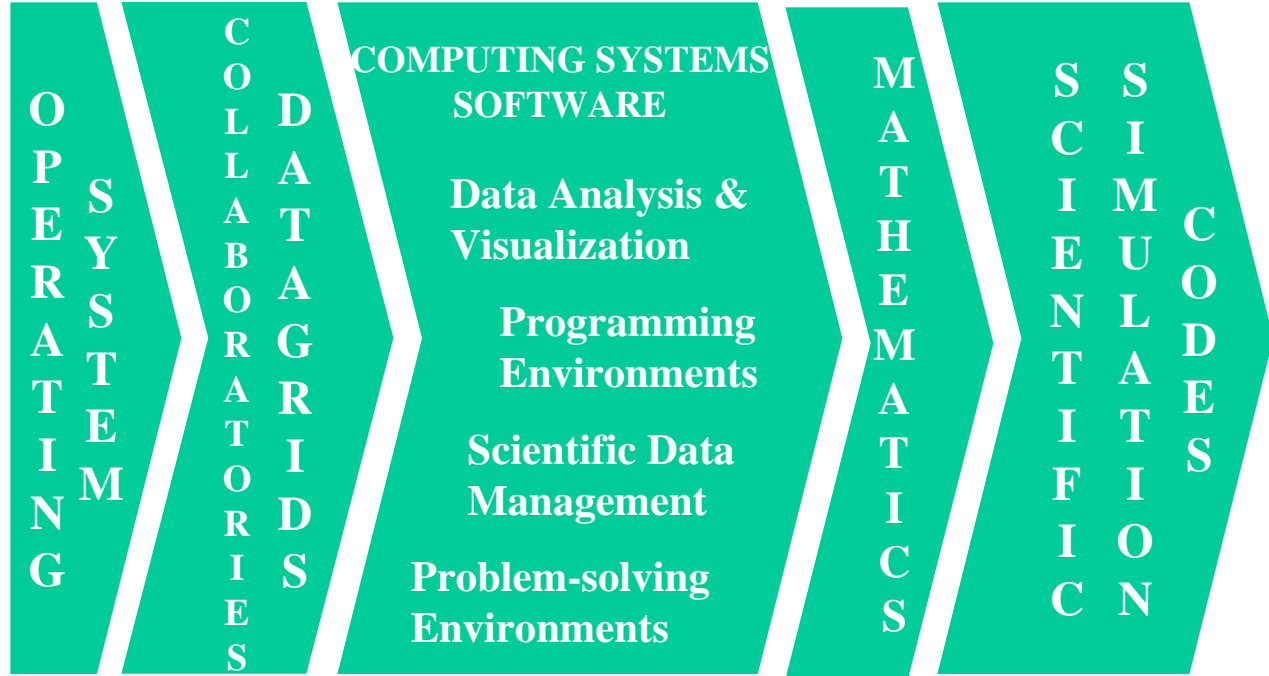
SciDAC Program Goal

An **integrated** program to:

(1) Create a new generation of Scientific Simulation Codes that take full advantage of the extraordinary computing capabilities of terascale computers.

(2) Create the Mathematical and Computing Systems Software to enable the Scientific Simulation Codes   to effectively and efficiently use terascale computers.

(3) Create a Collaboratory Software Environment to enable geographically separated scientists to effectively work together as a team and to facilitate remote access to both facilities and data.
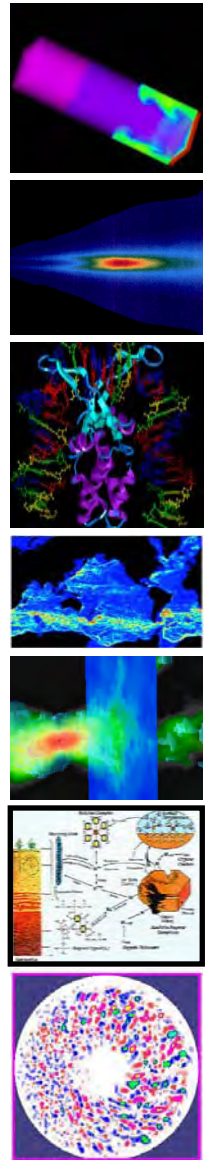
Scientific Computing Infrastructure
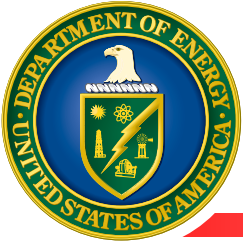
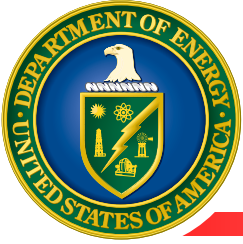**Hardware Infrastructure**

Software Infrastructure

O P E R A T I N G   S Y S T E M

C O L L A B O R A T O R I E S

D A T A   G R I D S

COMPUTING SYSTEMS SOFTWARE

Data Analysis & Visualization

Programming Environments

Scientific Data Management

Problem-solving Environments

M A T H E M A T I C S

S C I E N T I F I C

S I M U L A T I O N

C O D E S

ESnet BACKBONE Mid 1999

ASCR

BES, BER FES, HENP

FY2001 Budget for SciDAC

Program	2001 Appropriation
MICS	$37,443.
BES	1,931.
BER	8,000.
FES	3,000.
HEP	4,930.
NP	2,000.
Total	$57,304.

SciDAC Schedule for FY2001

Activity	Date
Publish "Notice of Intent"	December 4, 2000
Publish "Notices" (6)	December 27, 2000 (2)
Pre-proposal Deadline	January 31, 2001
Proposal Deadline	March 15, 2001
Review of Proposals Completed	May 3, 2001*
Award Recommendations	May 15, 2001*

* The objective of this aggressive schedule is to complete the selection of most awards in time for the June financial plan.
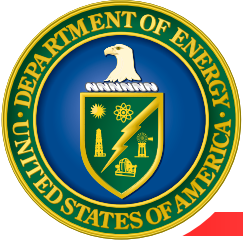
SciDAC Status

- Over 150 proposals received

- Several review panels completed in the past 2 weeks

- Overall quality of the proposals was very good to excellent

- Only about 1/4 - 1/3 of proposals can be funded

ASCR Plans for FY2001

- Enabling Technology Centers
  - Applied Mathematics ($8,000)
  - Computer Science ($8,000)
- Middleware and Network Research and Applications ($10,000)
  - Includes Collaboratories and Grid Pilot Projects
- Scientific Application Partnerships ($3,000)
- Computational Science Graduate Fellowships ($1,000)
- Advanced Computing Research Facilities ($2,000)
- Upgrade ESnet Services ($1,000)
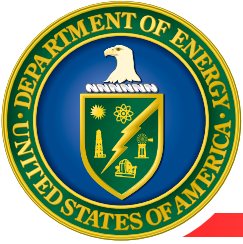
ASCR Program Status

National Collaboratories and High Performance Networks
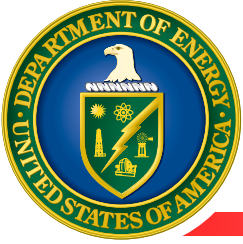
- 82 Preproposals Received

- 48 Proposals Received

  - High Performance Networks   12
  - Networking/Middleware   11
  - Middleware   12
  - Collaboratory Pilots   13

- Reviews held April 17-20, 2001
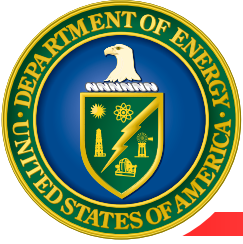
ASCR Program Status

Integrated Software Infrastructure Centers

- 36 Preproposals Received

- 16 Proposals Received

  - Computer Science   9

  - Mathematics   7
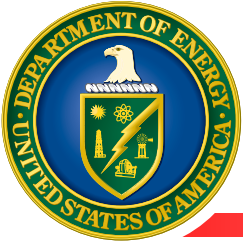
- Reviews Held April 18-19, 2001

BES Plans for FY2001

- Development of Scientific Simulation Methods and Codes for Terascale Computers ($1,931)
  - Understand and predict the energetics and dynamics of chemical reactions and the interaction between chemistry and fluid dynamics
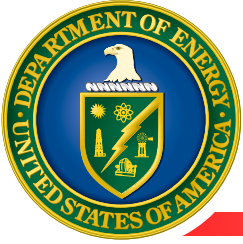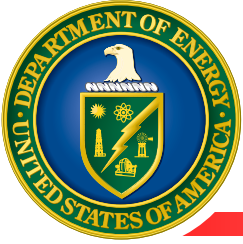
BES Program Status

Computational Chemistry

- 40 Preproposals Received
- 30 Proposals Received
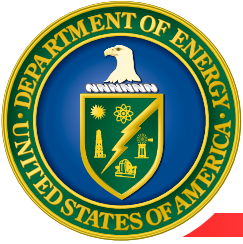- Review Scheduled for May 25, 2001

BER Plans for FY2001

- Development of Scientific Simulation Methods and Codes for Terascale Computers ($8,000)

  - Develop State-of-the-Science coupled GCM-based climate models to simulate and predict the earth's climate at both regional and global scales for decades to centuries, including levels of certainty and uncertainty

  - Develop flexible, efficient and extensible software frameworks to keep climate models at the cutting edge of scientific understanding and computational technology
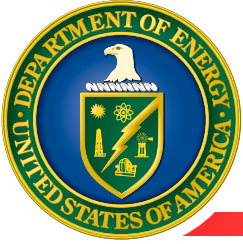
BER Program Status

Climate Change Prediction Program

- ~50 Prepropapsals Received
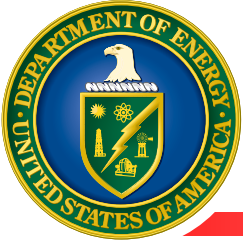- 41 Proposals Received
- Review Underway

FES Plans for FY2001

- Development of Scientific Simulation Methods and Codes for Terascale Computers ($3,000)
  - Predict microscopic turbulence and macroscopic stability in magnetically confined plasmas, including their effect on core and edge confinement
  - Predict the electromagnetic fields, beam dynamics, and other physical processes in heavy-ion accelerators for inertial fusion
  - Understand basic plasma science processes, such as electromagnetic wave-particle interactions and magnetic reconnection
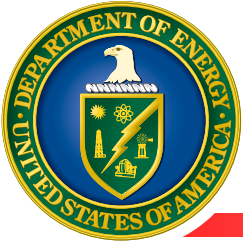
FES Program Status

Advanced Computing in Fusion and Plasma Science

- 20 Preproposals Received
- 13 Proposals Received
- Review held on April 23, 2001

HENP Plans for FY2001

- Development of Scientific Simulation Methods and Codes for Terascale Computers ($7,000)
  - Simulate beam dynamics and electromagnetic fields in particle accelerators in order to predict and optimize the behavior of accelerator components
  - Develop hardware and software infrastructure for large scale simulations of QCD, the fundamental theory governing strong interactions
  - Develop comprehensive models of supernovae explosions
  - Implement collaboratory pilot projects for large HENP experiments (with ASCR)

HENP Program Status

Advanced Computing in High Energy and Nuclear Physics Research

- 8 (+2) Preproposals Received
- 6 Proposals Received
  - Two of the proposals would implement parts of the vision for "Grid Computing"
- Review Held on April 20, 2001