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

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.
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

OPERATING SYSTEM
DATA Grids
COLLABORATORIES
COMPUTING SYSTEMS SOFTWARE
Data Analysis & Visualization
Programming Environments
Scientific Data Management
Problem-solving Environments

MATHEMATICS
Scientific Simulation

CODES
BES, BER
FES, HENP

ASCR
## FY2001 Budget for SciDAC

<table>
<thead>
<tr>
<th>Program</th>
<th>2001 Appropriation</th>
</tr>
</thead>
<tbody>
<tr>
<td>MICS</td>
<td>$37,443.</td>
</tr>
<tr>
<td>BES</td>
<td>1,931.</td>
</tr>
<tr>
<td>BER</td>
<td>8,000.</td>
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<tr>
<td>FES</td>
<td>3,000.</td>
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<tr>
<td>HEP</td>
<td>4,930.</td>
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<tr>
<td>NP</td>
<td>2,000.</td>
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<tr>
<td>Total</td>
<td>$57,304.</td>
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</tbody>
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### SciDAC Schedule for FY2001

<table>
<thead>
<tr>
<th>Activity</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Publish “Notice of Intent”</td>
<td>December 4, 2000</td>
</tr>
<tr>
<td>Publish “Notices” (6)</td>
<td>December 27, 2000 (2)</td>
</tr>
<tr>
<td>Pre-proposal Deadline</td>
<td>January 31, 2001</td>
</tr>
<tr>
<td>Proposal Deadline</td>
<td>March 15, 2001</td>
</tr>
<tr>
<td>Review of Proposals Completed</td>
<td>May 3, 2001*</td>
</tr>
<tr>
<td>Award Recommendations</td>
<td>May 15, 2001*</td>
</tr>
</tbody>
</table>

* 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)
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
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 Preproposals 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