

Advanced Scientific Computing Research

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An Update

ASCAC Meeting
May 2-3, 2002
Washington, DC

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Advanced Scientific Computing Research
Office of Science

<http://www.sc.doe.gov/production/octr/mics/index.html>



Mission

Advanced Scientific Computing Research

Discover, develop, and deploy the computational and networking advances that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex physical, chemical, and biological phenomena important to the Department of Energy (DOE).

support a broad research portfolio in advanced scientific computing – applied mathematics, computer science, networking and collaboratory software

operate supercomputers, a high performance network, and related facilities.



Principles and Attributes

Advanced Scientific Computing Research

- **MICS will advance DOE science and missions through**
 - world-class applied mathematics and computer science research,
 - innovative software technologies
 - cost-effective high-performance computational and networking resources
- **Strategies-**
 - review MICS management processes and MICS portfolio
 - expand applied math and computer science base research
 - develop research partnerships with all Office of Science programs
 - acquire/deploy high-end computational and network resources in a systematic manner
 - enhance coordination with other agencies
- **Values-**
 - excellence and innovation in everything we do
 - consistent high standards to all existing and prospective research performers
 - the best research and PIs, regardless of affiliation



Major Events

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- **FY 2001**
 - Initiated software infrastructure portion of SciDAC
 - Initiated computational biology research efforts
 - Upgraded NERSC to 5 teraflops
 - Acquired IBM Power 4 Hardware for evaluation/scaling studies
- **FY 2002**
 - Issued research call for Early Career Principal Investigators
 - Conducted Genomes to Life workshops with BER
 - Conducted the Mission Computing Conference
 - Organized workshops with BES (May 10-11, 2002) and FES (May 23-24, 2002)
 - Approved LBNL proposal to manage and to operate NERSC
 - Convened first SciDAC Principal Investigator Meeting
- **FY 2003 Plans**
 - Launch GTL computational component, in partnership with BER
 - Initiate computational nanoscience partnership with BES (SciDAC)
 - Provide topical, high performance computing resources (SciDAC)
 - Develop/propose SC strategy for high-performance networks (August 13-15, 2002)



Base Research Program New Directions for FY2002

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Early Career Principal Investigator

- 132 Grant applications submitted;
 - Applied mathematics: 63
 - Computer science: 47
 - Network research: 22
- Award schedule
 - Peer reviews completed: June 20, 2002
 - Decisions made: July 1, 2002; (15-25 awards expected)
 - Research efforts started: September 1, 2002

HBCU Initiative

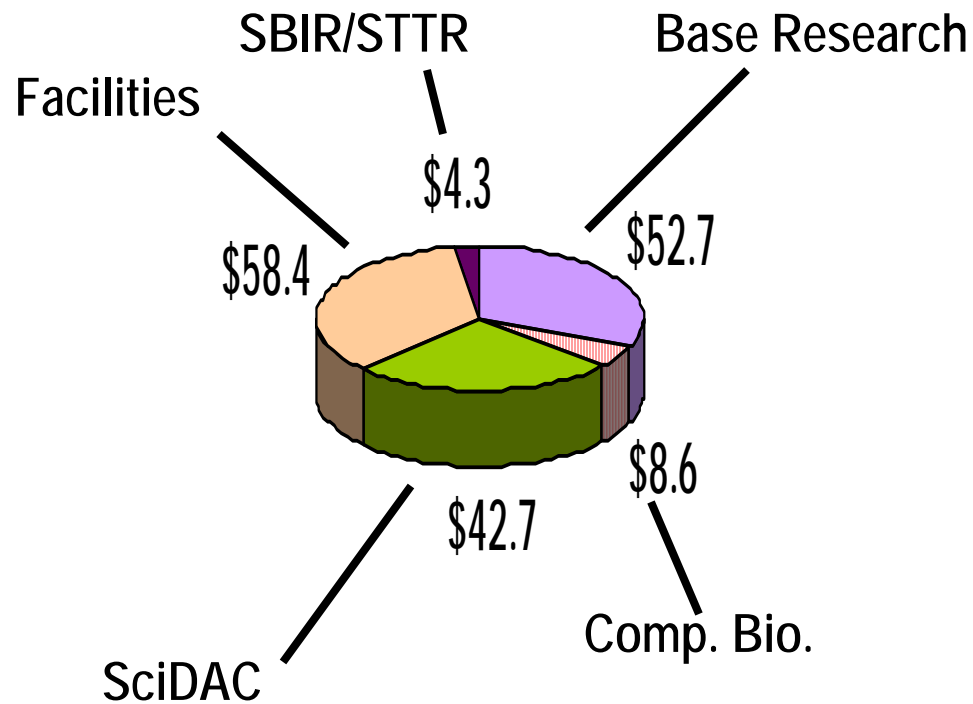
- Goal: Increase HBCU participation in ASCR research
 - Visits to Howard, Morgan State and other HBCUs scheduled
 - Pilot program initiated: Research Alliance for Minorities
 - Outreach coordinated with Office of Science Education program



MICS Budget Request (\$ in millions)

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FY2003- \$166.6



Enhancements over FY2002

- Computational Biology +\$5.6
- SciDAC +\$5.3
- Facilities +\$1.3



Opportunities

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Topical Computing Centers

- Effective and efficient computing resources optimized for a set of scientific applications
- Focal points for scientific research communities
- A key element in the SciDAC strategy

Strategic Research Partnerships

- Goal: Bring tera-scale simulation capability to bear on all major science issues facing the Office of Science
 - Genomes to Life, Computational Nanoscience, Fusion plasma simulation, QCD, astrophysics, etc.

Develop/Implement strategy for high-performance computing and networking

Support base research activities at levels needed to meet enhanced expectations



Staff

Advanced Scientific Computing Research

- Ed Oliver, Associate Director for Advanced Scientific Computing Research;
Acting CIO, Office of Science
- Dan Hitchcock, Senior Technical Advisor
- Linda Twenty, Program Analyst & Financial Specialist
- Melea Baker, Secretary- Office Automation

- Walt Polansky, Acting Director MICS*
- Gary Johnson, ACRTs, Computational Biology
- Fred Johnson, Computer Science
- William (Buff) Miner, NERSC & Scientific Applications
- Thomas Ndousse-Fetter, Network Research
- Kimberly Rasar, Senior Info. Tech. (SciDAC)
- Chuck Romine, Applied Mathematics (Base* & SciDAC)
- Mary Anne Scott, Collaboratories
- George Seweryniak, ESnet
- John van Rosendale, Computer Science- Visualization and Data Management

- Jane Hiegel, Secretary- Office Automation
- Susan Kilroy, Office Automation Assistant

- * Vacancies- (2): Applied Mathematics Program Manager (Base);
Director, MICS



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Back-up Slide



Department of Energy Mission and Priorities

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- Guaranteeing the safety and reliability of the nuclear stockpile;
- Ensuring the R&D and production plans support the Administration's nuclear strategy;
- Resolving the threat of weapons of mass destruction;
- Provide safe, efficient and effective nuclear power for the Navy;
- Ensuring energy security through infrastructure protection;
- Implementing the President's National Energy Plan;
- Directing R&D budgets to innovative new ideas while ensuring applications of mature technologies;
- Exploring new energy sources with dramatic environmental benefits;
- Supporting Homeland Defense through a focus on the threats of weapons of mass destruction posed by terrorist or nation states

Strong Relevance to ASCR FY2003 Budget Request