Mission:

- Deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.
Staff

Office of Advanced Scientific Computing Research
- Ed Oliver, Associate Director for Advanced Scientific Computing Research
- Dan Hitchcock, Senior Scientific Advisor
- Linda Twenty, Senior Budget & Financial Specialist
- Melea Baker, Administrative Specialist

Mathematical, Information and Computational Sciences Division
Ed Oliver, Acting Director MICS
- Gary Johnson, ACRTs, Computational Biology
- Fred Johnson, Computer Science
- William (Buff) Miner, NERSC & Scientific Applications
- Thomas Ndousse-Fetter, Network Research
- Chuck Romine, (on detail to OSTP) Applied Mathematics
- Mary Anne Scott, Collaboratories
- George Seweryniak, Esnet
- John van Rosendale, Computer Science- Visualization and Data Management
- Jane Hiegel, MICS Secretary
- Division Secretary
(Total Vacancies = 3)
ASCR Program Overview

**External to SC**

- **Underlying Technologies**
  - Hardware
  - Software
  - Networking

- **Fundamental Research**
- **SciDAC**
- **Partnerships**
- **Science**

**Enabling Science through Computing**

- **Applied Mathematics**
- **Computer Science**
- **Advanced Computing Software Tools / Integrated Software Infrastructure Centers**
- **Scientific Application Partnerships**

**Next Generation Architecture**

- **Computer Science**
- **Research and Evaluation Computers**
- **Leadership Class Computer**

**High Performance Network Environment for Science**

- **Networking**
- **Collaboratory Tools**
- **Collaboratory Pilots**

**Core Facilities**

- **High Performance Production Computing Capability**
- **Energy Sciences Network (ESnet)**

**BES, BER, FES, HEP, NP**

- **Applications, e.g.**
  - Materials Sciences
  - Chemical Sciences
  - Combustion Modeling
  - Biology - GEE
  - High Energy Physics
  - Nuclear Physics
  - Fusion Energy
  - Global Climate

- **Leadership in High Performance Computing**
- **Access to Facilities**
- **Link Researchers**
Scientific Discovery Through Advanced Computation (SciDAC)

Brings the power of terascale computing to science

Hardware Infrastructure

- Operating System
- Architecture

Software Infrastructure

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

ASCRA

State-of-the-art electronic collaboration tools will facilitate access to these tools to bring simulation to a level of parity with theory and experiment in the scientific enterprise.
The Next Generation Computer Architecture for Science and Industry (NGA) research activity is an integral part of an Office of Science strategy to acquire additional advanced computing capability to support existing users in the near term and to initiate longer-term research and development on next generation computer architectures. NGA research and testbed activities will lead to the development of potential Leadership Class Machines that enable solutions for scientific and industrial problems beyond what would be attainable through a continued simple extrapolation of current computational capabilities.

The NGA plays a critical role in the implementation of the interagency plan developed by the High End Computing Revitalization Task Force (HECRTF), which was chartered by the President’s Science Advisor.

In FY05 the NGA will:

- Complete the evaluation of initial NGA Research and Evaluation prototype – the Cray X1 at ORNL;
- Continue work with the scientific application community and industrial researchers and the vendor community to significantly improve understanding of interactions between high-end system architecture and key application performance, in partnership with DARPA, NNSA, and NSA;
- Continue the academic, laboratory, and vendor research program on scalable technologies for future generations of operating systems and runtime environments that was initiated in FY04;
- Continue the strong partnership with the DARPA High Productivity Computing Systems program to enable the development of next generation computer hardware for science; and
- Initiate Leadership Class Computer through peer reviewed competition.
Multiscale Mathematics

- Across the Office of Science many applications involve multiscale physics / biology / chemistry
  - Climate: Regional effects on global climate
  - Biology: Timescales from vibrational frequencies to ligand transport time
  - High-Energy Physics: supernova modeling involves many length/time scales
  - Combustion: fast chemical reaction rates to slow-moving flame fronts
  - Fusion: From the electron gyroradius to the connection length
- Current models assume separation of length/time scales, which fails in practice
- Roadmap to be developed in Workshops, the first in May 2004.
ASCR/MICS Budget

<table>
<thead>
<tr>
<th>Fiscal Year</th>
<th>Request</th>
<th>Appropriation</th>
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<tbody>
<tr>
<td>2003</td>
<td>$163,557,000</td>
<td>$160,367,000**</td>
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<td>2004</td>
<td>$170,490,000</td>
<td>$198,818,000*</td>
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<tr>
<td>2005</td>
<td>$204,340,000</td>
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</table>

* Following General Reduction & Omnibus Rescission

** Following General Reduction & Omnibus Rescission, SBIR Removed
INCITE: Expanding the Impact of NERSC on U.S. Science

Innovative and Novel Computational Impact on Theory and Experiment

10% of NERSC capability made available to the scientific community for high impact science. No requirement for direct relationship to Office of Science programs.
Overview of the INCITE Proposals

- 4,500,000 CPU hours available (10% of NERSC Capability)
- 53 proposals received
- 130,508,660 CPU hours requested
- 65% from U.S. academic institutions
- 12 different scientific disciplines
- 62% for research not funded by DOE
Compute Facilities and Testbeds Timeline

- Experiment
- R&E Prototype
- Leadership-Class
- High Performance Production Capability
- High Performance Capacity
- Desktop

Year 1 to Year 10
Research to Enable New Frontiers in Science through Simulation

- The mathematics of complex and multiscale systems;
- Ultrascalable algorithms for petascale systems;
- The computer science to enable advanced computers; and
- The computer science to transform petabytes of data into knowledge.
Science applications and specialized experimental facilities are n-way interconnected to terascale computing, petascale storage, high-end visualization, and remote collaborators in a seamless environment that provides the performance level required to move science, especially large-scale science, to a new regime—rapid scientific progress through the interplay of theory simulation, and experiment.
Providing high performance computing and network facilities;

Maintaining world-class research effort in applied mathematics, computer science, and computer networks;

Effective partnerships with applications scientists in all of the Offices in SC;

Effective partnerships with other Federal Agencies;

Accelerating transition from research to application; and

Long-Term support of software.
ASCR in Relationship to Federal IT Research

President’s Information Technology Advisory Committee (PITAC)

White House
OSTP/OMB

National Science & Technology Council (NSTC)

Senior Principal’s Group for IT

Interagency Working Group on IT R&D (IWG/ITR&D)

Participating Agencies
AHRQ, DARPA, DOE, EPA, NASA, NIST, NOAA, NSA, NSF, OSD/URI

National Coordination Office for Computing, Information and Communications (NCO/CIC)

HECC
High End Computing and Communication Coordinating Group

LSN
Large Scale Networking Coordinating Group

HCl&IM
Human Computer Interface & Information Management Coordinating Group

HCSS
High Confidence Systems & Software Coordinating Group

SDP
Software Design & Productivity Coordinating Group

SEW
Social, Economic & Workforce Implications of IT and IT Workforce Development Coordinating Group

Joint Engineering Team (JET)

Network Research Team (NRT)

Middleware and Grid Infrastructure Coordination (MaGIC)

DOE Direct Involvement
Co-Chair of Interagency High End Computing Revitalization Task Force;
Signed Memorandum of Understanding with NNSA, DOD-DDR&E, NSA, and DARPA for joint planning of high end computing research activities;
Ongoing joint high end computing research activities with NNSA, DARPA, and NSA
Co-Chair of Interagency Large Scale Networking Coordination Group and all 3 teams: Joint Engineering (JET), Network Research (NRT), and Middleware and Grid Infrastructure Coordination (MAGIC).
Workshops and Reports

- High Performance Network Planning Workshop, August 2002
  - http://www.doecollaboratory.org/meetings/hpnw/
- Blueprint for Future Science Middleware and Grid Research and Infrastructure, August 2002
- DOE Science Network Meeting, June 2003
  - http://gate.hep.anl.gov/may/ScienceNetworkingWorkshop/
- DOE Science Computing Conference, June 2003
  - http://www.doe-sci-comp.info
- Science Case for Large Scale Simulation, June 2003
  - www.pnl.gov/scales/
- Workshop on the Road Map for the Revitalization of High End Computing
  - http://www.cra.org/Activities/workshops/nitrd/
- Cyberinfrastructure Report
- ASCR Strategic Planning Workshop
  - http://www.fp-mcs.anl.gov/ascr-july03spw
BACKUP
Research to Enable New Frontiers in Science through Networks

- End-to-end performance
- High-Performance Middleware
- Integrated testbeds and networks
INCITE Proposals by CPU Hours Requested
(Total of 130,508,660 hours requested)
INCITE Details

INCITE Proposals by Funding Source

- 32 Not DOE Funded
- 20 DOE Funded

[Legend: Blue = DOE Funded, Red = Not DOE Funded]
Algorithm Scaling with Problem Size
Determines the Size Problem that can be Solved!

Algorithms determine what fraction of peak performance is delivered to science

Graphs showing the relationship between problem size and performance, with different scaling notations and performance metrics.
“Forefront computational capabilities” to “extend the frontiers of science” require

- Well-posed mathematical models (e.g., PDEs)
- Mathematical analysis of model behavior
- Solvable discrete versions (grid generation and discretization)
- Efficient algorithms for solving the discretized models
- Predictability analysis and uncertainty quantification for model reduction and to determine levels of confidence in the results
- Engineering design optimization, discrete optimization problems, constrained optimization problems
- New areas (dynamical systems, multiresolution analysis, multiscale mathematics, scalable algorithms) dictated by need and opportunity
Petascale systems by 2010 (100,000+ processors)

Very challenging architecture diversity – X1, Red Storm, BG/L, DARPA HPC systems

Reliability/fault management

Software engineering

CS Hardware Testbeds
Opportunities

- SW framework (probably CCA-based) for visualization; research
- Appropriate research infrastructure;
- Petabyte-scale data;
- Complex data structures;
- Interaction with Network Environment Research
Opportunities

- End-to-end performance
  - Multi-domain
  - Ultra high-speed transport protocol
  - Network measurement and prediction

- Cyber security
  - Scalable distributed authentication and authorization systems
  - Ultra high-speed network components

- High-Performance Middleware
  - Network caching and computing
  - Real-time collaborative control and data streams
  - Fault-tolerance, error detection/correction

- Integrated testbeds and networks
  - Network research to accelerate advanced technologies
  - Experimental deployment of high-impact applications
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