U.S. Department of Energy's
Office of Science

Advanced Scientific Computing Research Program

U.S. Department of Energy

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Advanced Scientific Computing Advisory Committee Meeting

April 5 and 6, 2004

Dr. C. Edward Oliver
Ed.Oliver@science.doe.gov
www.science.doe.gov/ascr/

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Advanced Scientific Computing Research (ASCR)

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.

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ASCR in Relationship to Office of Science

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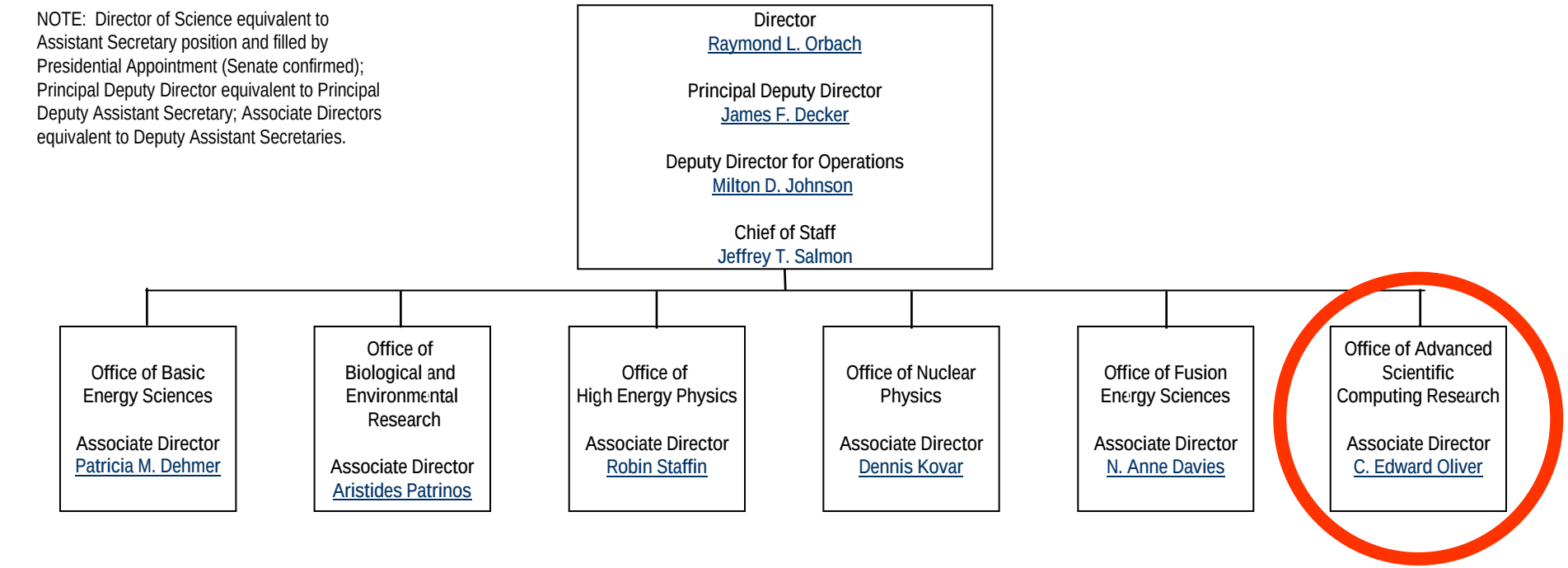
NOTE: Director of Science equivalent to Assistant Secretary position and filled by Presidential Appointment (Senate confirmed); Principal Deputy Director equivalent to Principal Deputy Assistant Secretary; Associate Directors equivalent to Deputy Assistant Secretaries.



www.science.doe.gov

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)

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ASCR Program Overview

External to SC | ASCR | BES, BER, FES, HEP, NP

Underlying Technologies → Fundamental Research → SciDAC → Partnerships → Science

- Hardware
- Software
- Networking

Enabling Science through Computing

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

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

Next Generation Architecture

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

•Leadership in High **Performance Computing**

High Performance Network Environment for Science

- Networking
- Collaboratory Tools
- Collaboratory Pilots

- Access to Facilities
- Link Researchers

Core Facilities

High Performance Production Computing Capability

Energy Sciences Network (ESnet)

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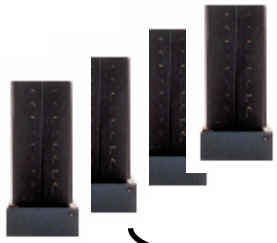
Scientific Discovery Through Advanced Computation (SciDAC)

Brings the power of terascale computing to science

Hardware Infrastructure

Software Infrastructure



OPERATING SYSTEM

ARCHITECTURE RESEARCH

COMPUTING SYSTEMS SOFTWARE

Data Analysis & Visualization

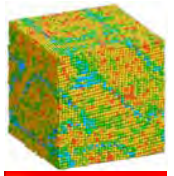
Programming Environments

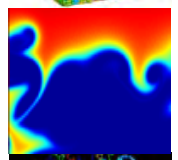
Scientific Data Management

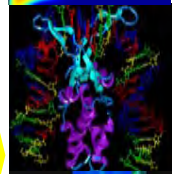
Problem-solving Environments

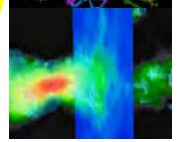
MATHEMATICS

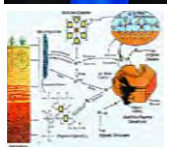
SCIENTIFIC SIMULATION CODES











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BES, BER FES, HENP

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.

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Next Generation Computer Architecture (NGA)

[FY 2004 $ 37.8M, FY 2005 $ 38.2M]

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.

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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.

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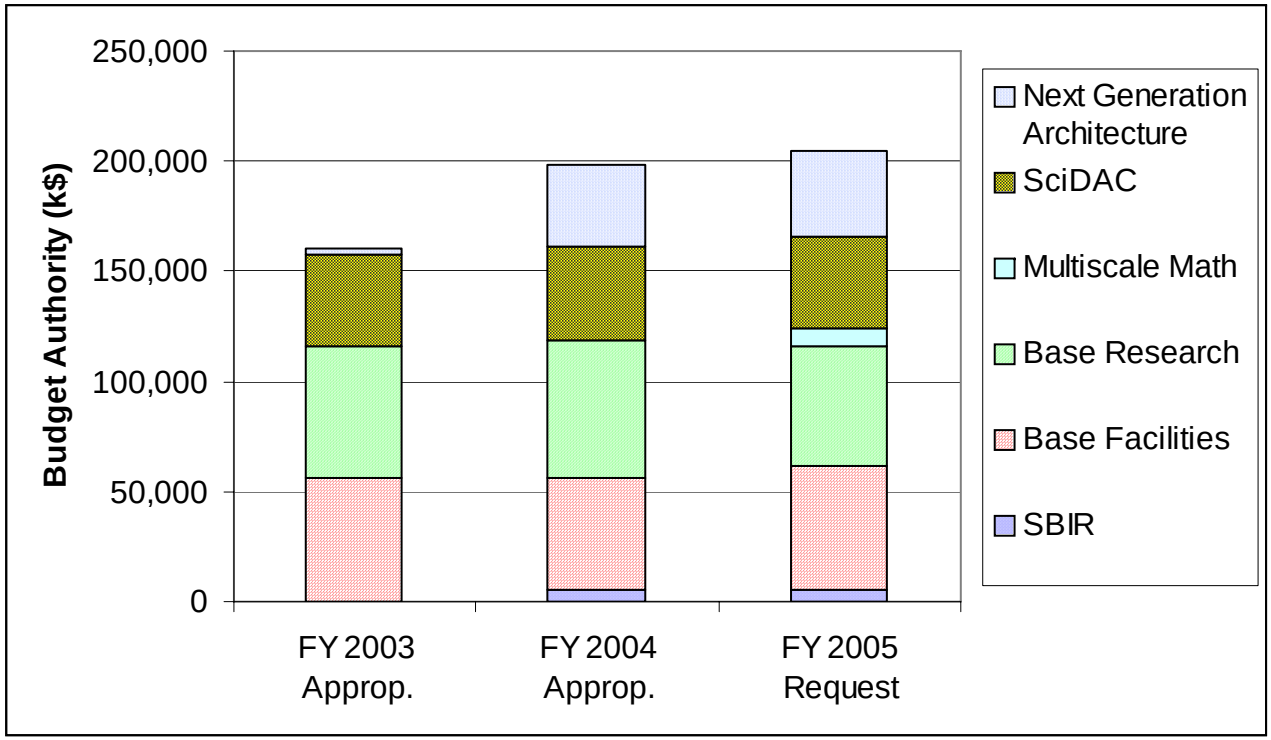
ASCR/MICS Budget



Fiscal Year	Request	Appropriation
2003	$163,557,000	$160,367,000**
2004	$170,490,000	$198,818,000*
2005	$204,340,000	TBD

* Following General Reduction & Omnibus Rescission

** Following General Reduction & Omnibus Rescission, SBIR Removed

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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

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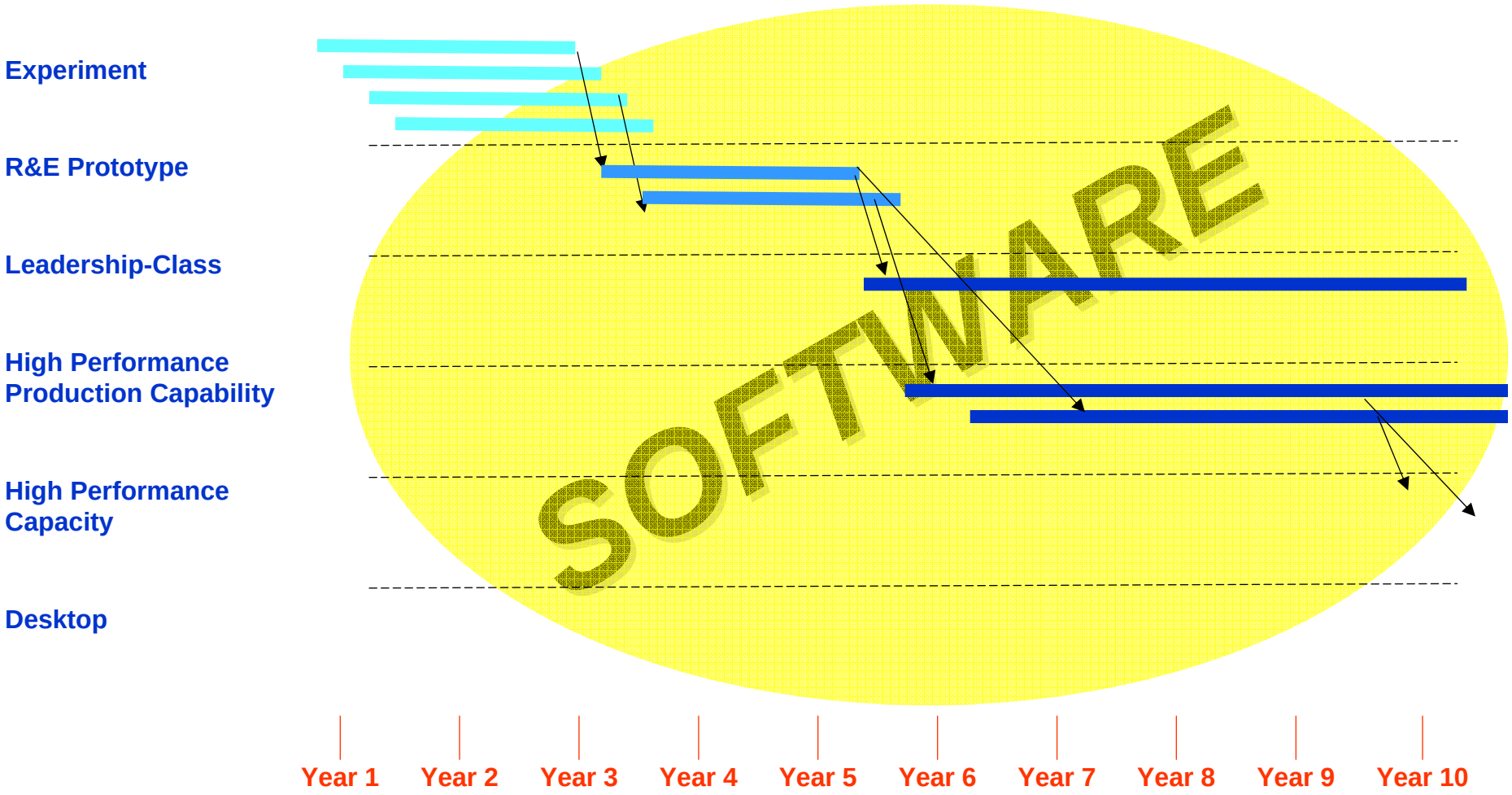
Compute Facilities and Testbeds
Timeline



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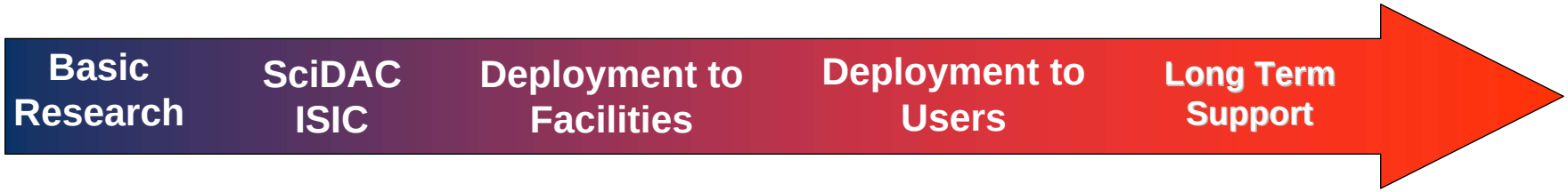
Research to Enable New Frontiers in Science through Simulation

- 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.



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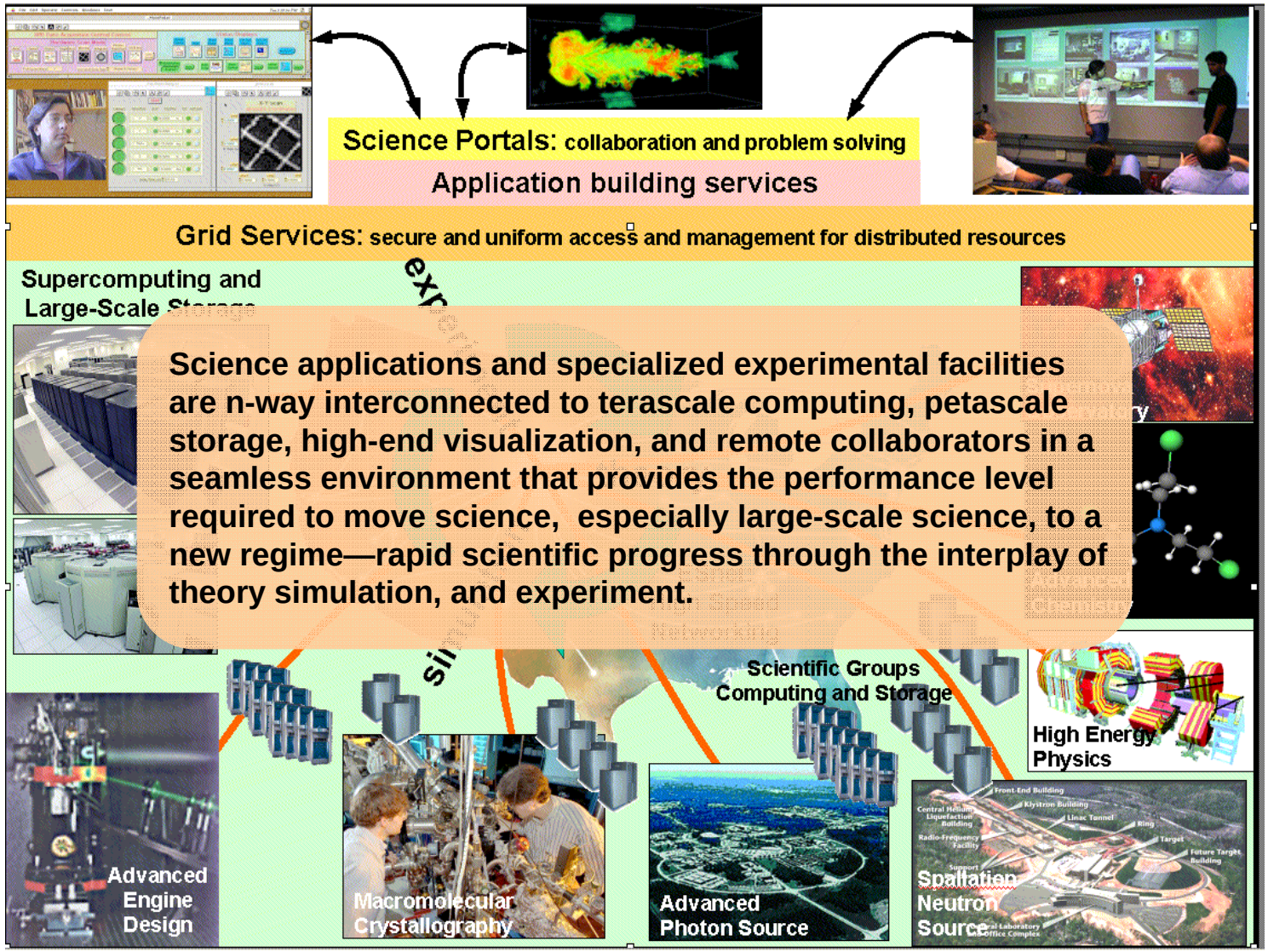
Network Environment Research



Strategic Issues for ASCR
Enabling World Leadership in Science

- 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.

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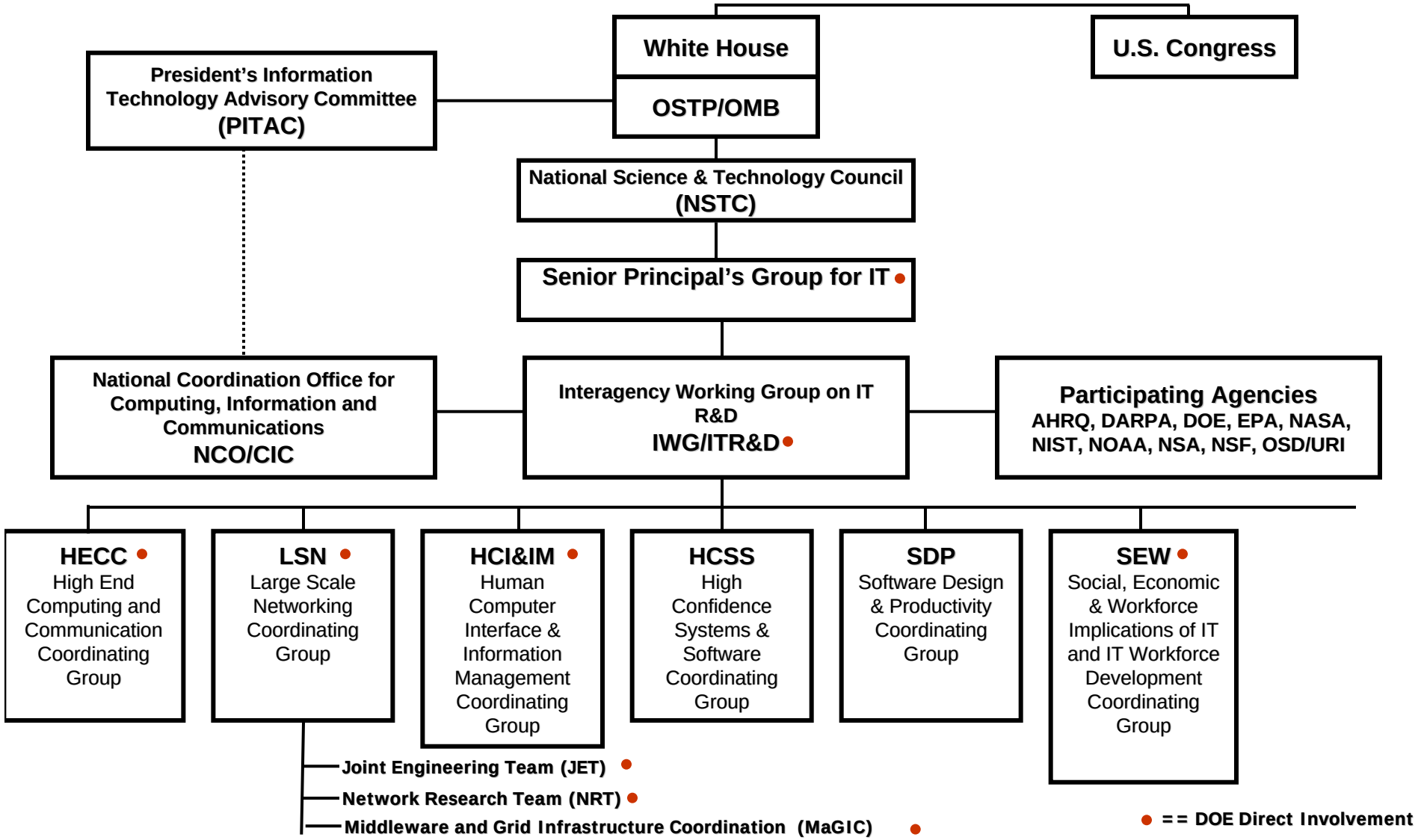
ASCR in Relationship to Federal IT Research



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ASCR Inter-Agency Coordination Overview

- 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/hpnpw/
- Blueprint for Future Science Middleware and Grid Research and Infrastructure, August 2002
  - http://www.nsf-middleware.org/MAGIC/default.htm
- 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
  - http://www.cise.nsf.gov/evnt/reports/toc.htm
- ASCR Strategic Planning Workshop
  - http://www.fp-mcs.anl.gov/ascr-july03spw

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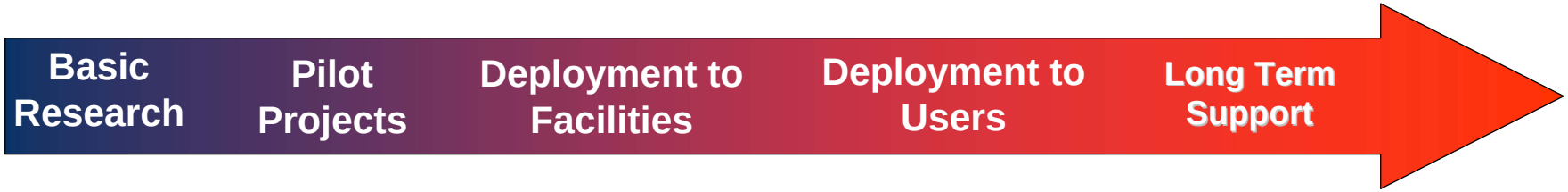
Research to Enable New Frontiers in Science through Networks

- End-to-end performance
- High-Performance Middleware
- Integrated testbeds and networks



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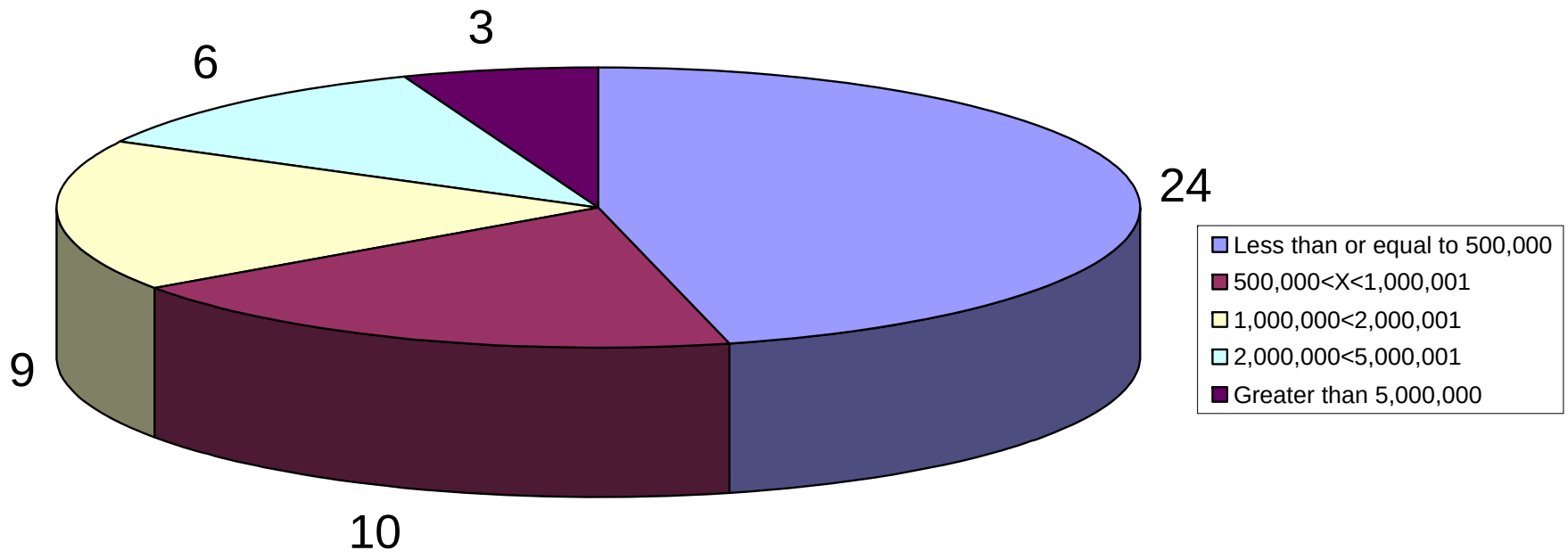
INCITE Details

INCITE Proposals by CPU Hours Requested
(Total of 130,508,660 hours requested)



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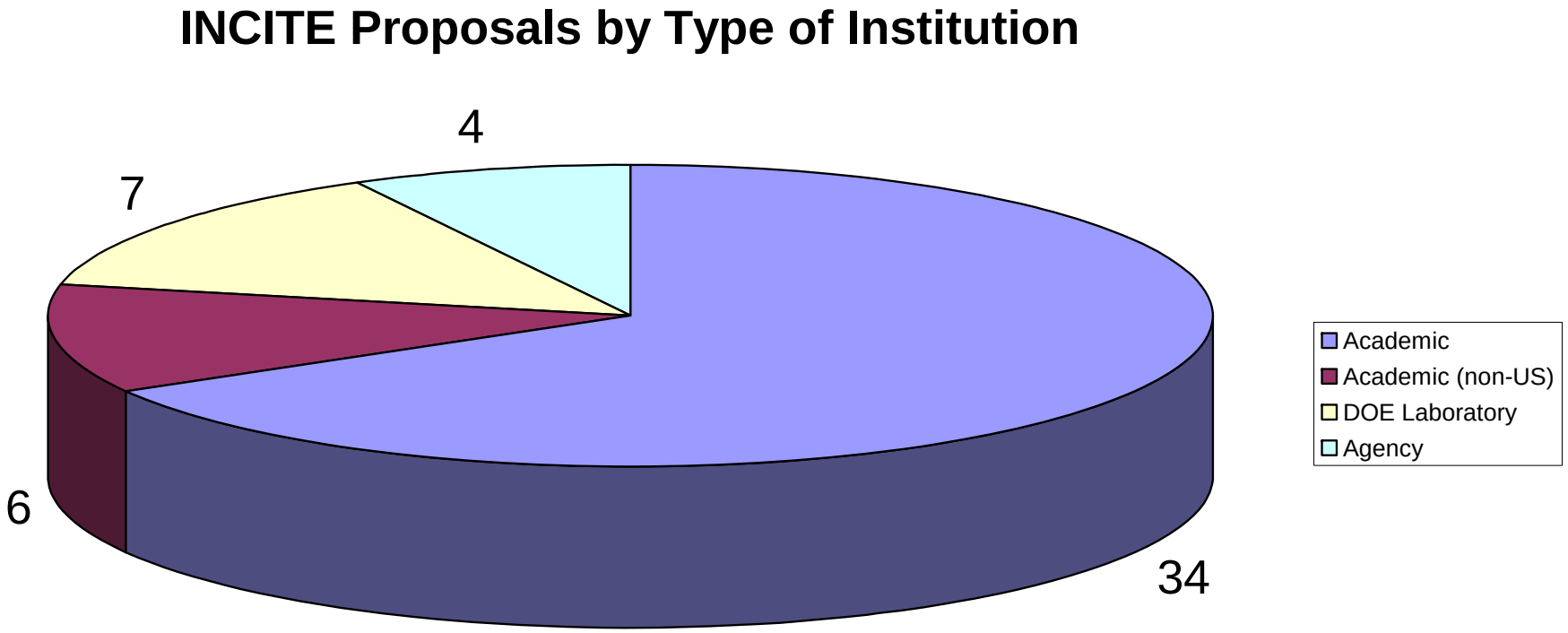

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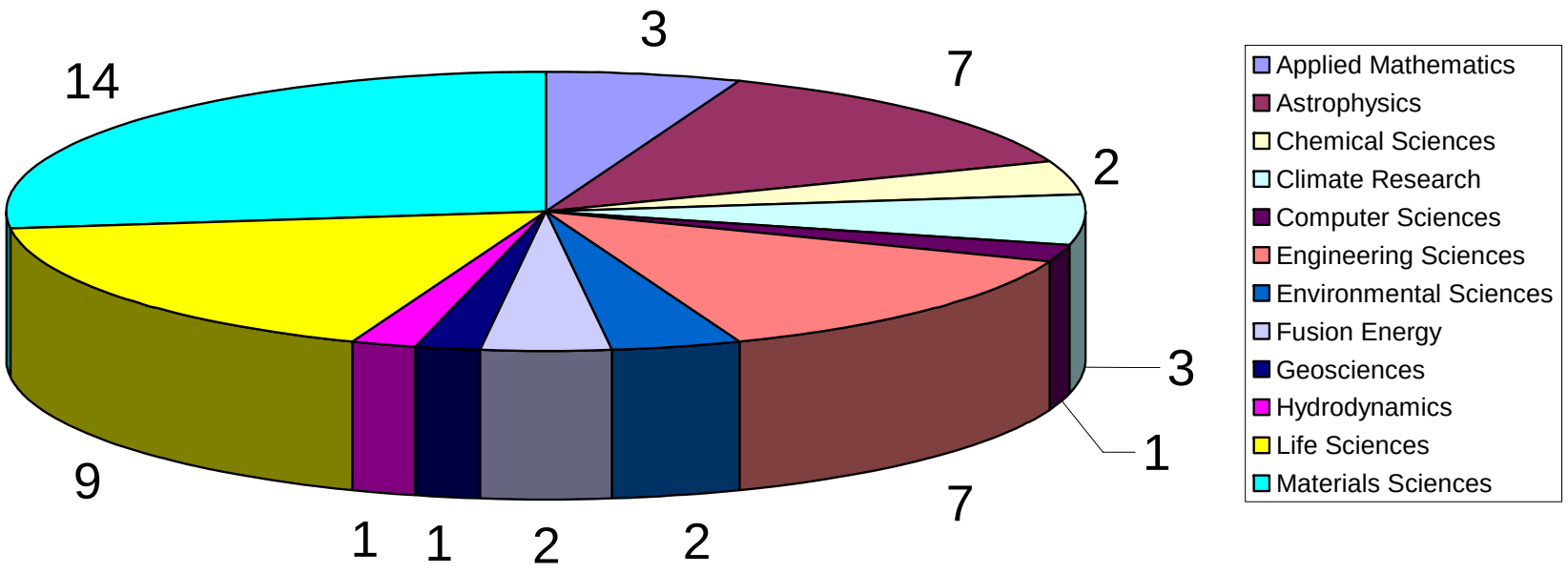
INCITE Details

INCITE Proposals by Scientific Discipline



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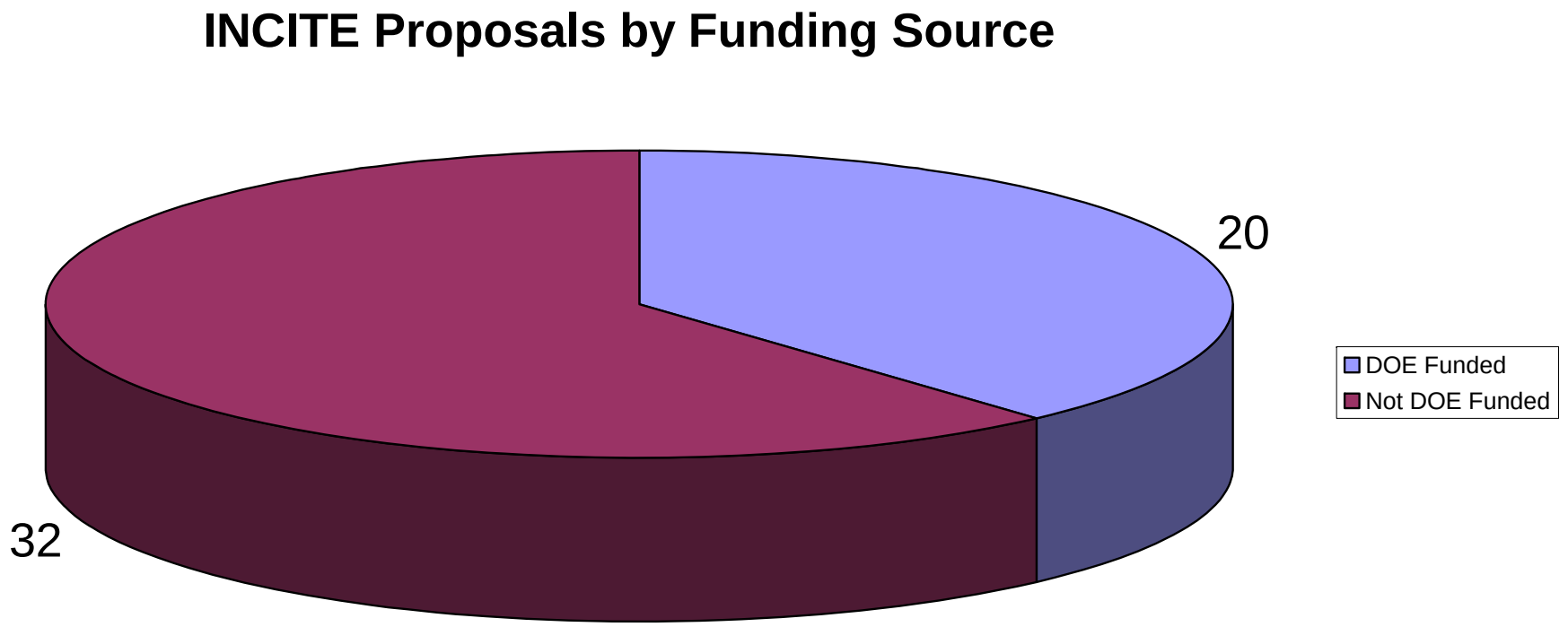

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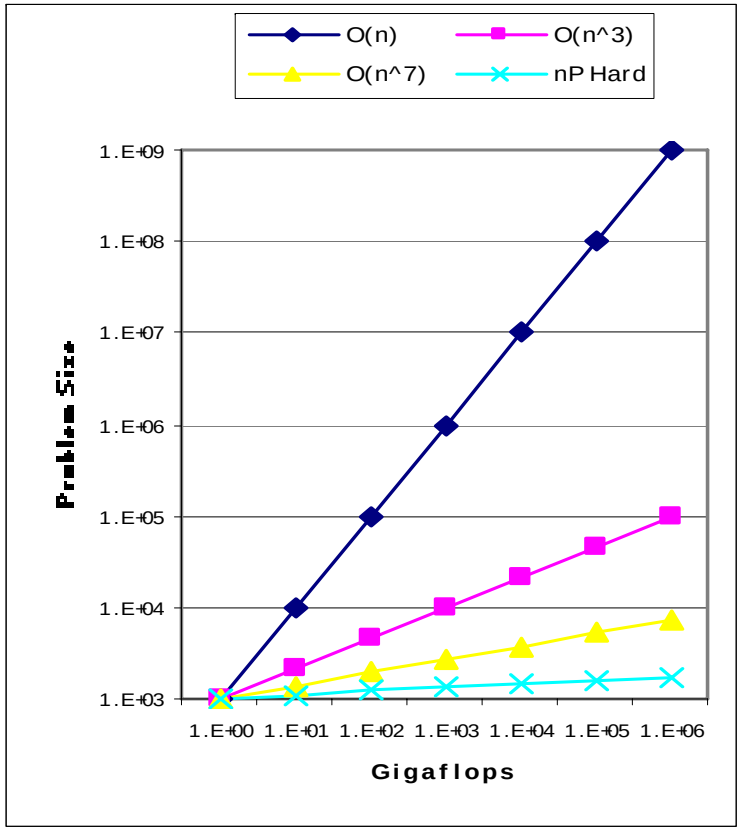
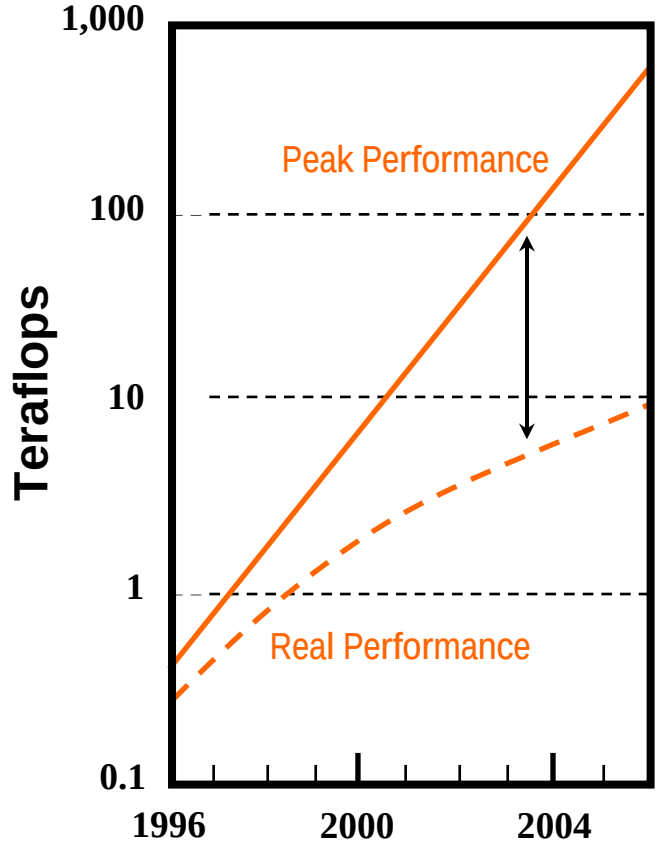
Applied Math Challenges

Algorithm Scaling with Problem Size Determines the Size Problem that can be Solved!



Algorithms determine what fraction of peak performance is delivered to science



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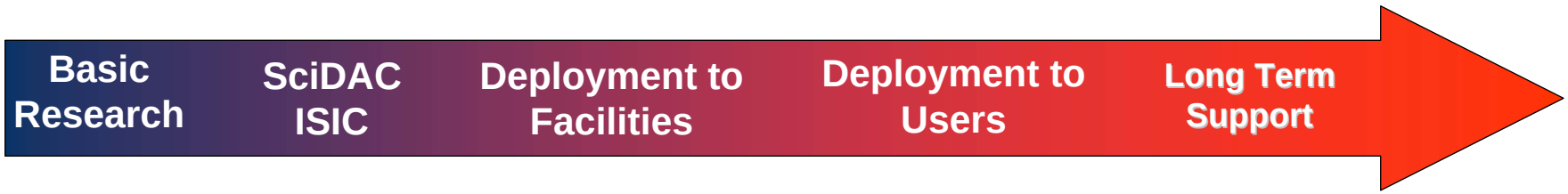
Applied Mathematics
Contribution to ASCR Strategic Goal

- "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



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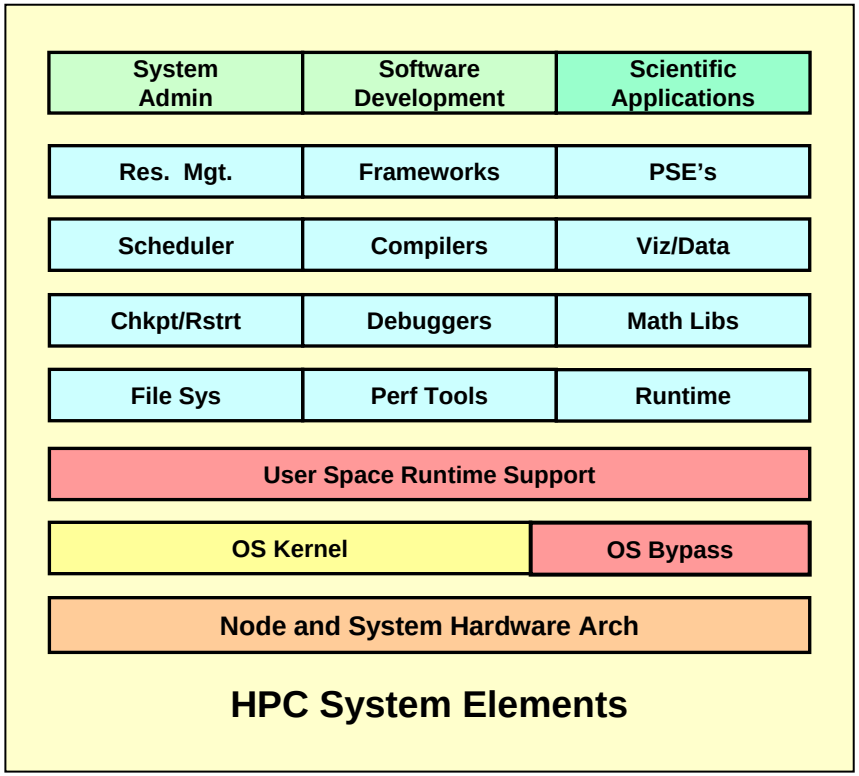
Computer Science Research
Systems Software & Tools



HPC System Elements

Opportunities

- 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

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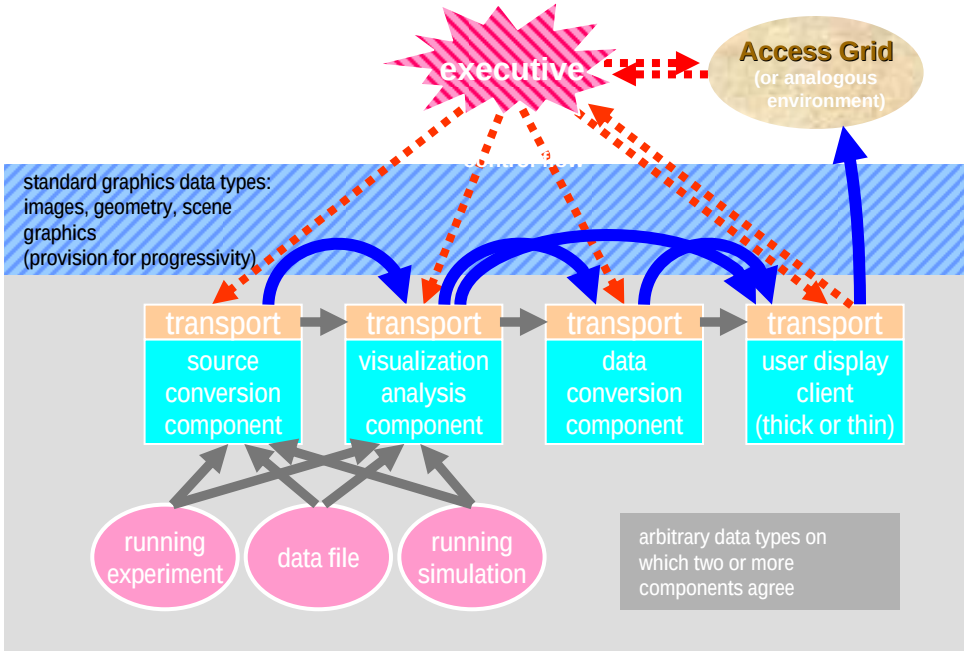
Computer Science Research
Data Management & Visualization



Opportunities

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

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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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