U.S. DEPARTMENT OF ENERGY | Office of Science

# News from the Office of Science

Advanced Scientific Computing Advisory Committee

August 11, 2009

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Director, Office of Science
U.S. Department of Energy

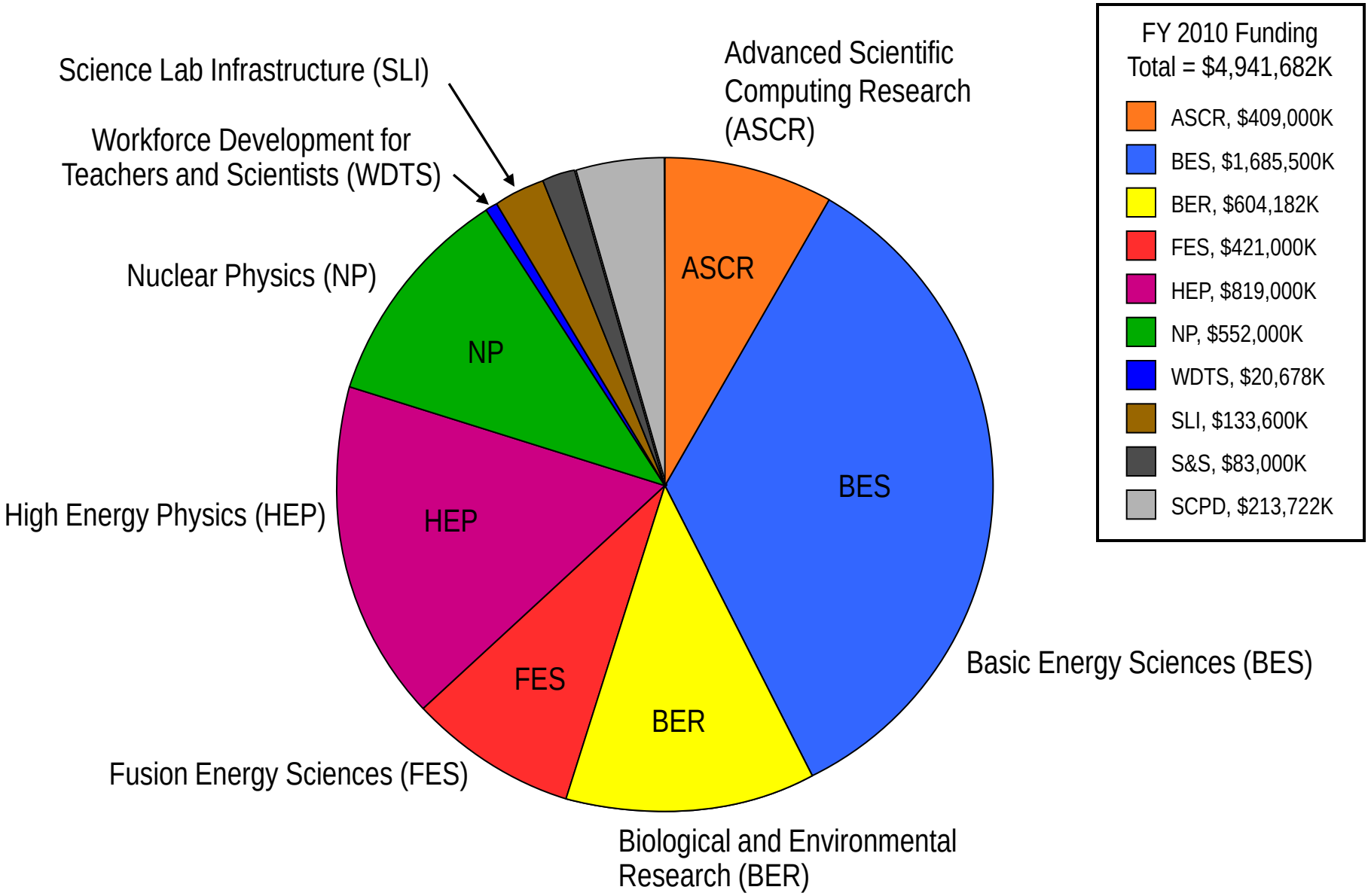
# DOE's Office of Science

**The Office of Science is one of the nation's largest supporters of peer-reviewed basic research, providing 40% of Federal support in the physical sciences and supporting ~25,000 Ph.D.s, graduate students, undergraduates, engineers, and support staff at more than 300 universities and at all 17 DOE laboratories.**

**Three themes describe the work supported by the Office of Science:**

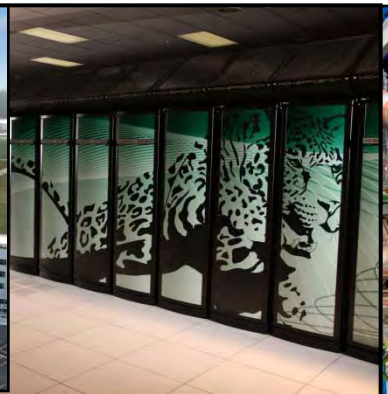
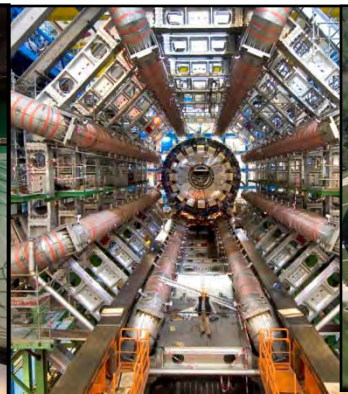
- **Science for discovery**
  - Unraveling Nature's deepest mysteries—from the study of subatomic particles; to atoms and molecules that make up the materials of our everyday world; to DNA, proteins, cells, and entire natural ecosystems
- **Science for national need**
  - Advancing a clean energy agenda through basic research on energy production, storage, transmission, and use
  - Advancing our understanding of the Earth's climate through basic research in atmospheric and environmental sciences and in climate modeling
  - Supporting DOE's missions in national security
- **National scientific user facilities, the 21st century tools of science**
  - Providing the Nation's researchers with the most advanced tools of modern science including accelerators, colliders, supercomputers, light sources and neutron sources, and facilities for studying the nanoworld, the environment, and the atmosphere

# Office of Science Programs



# User Facilities

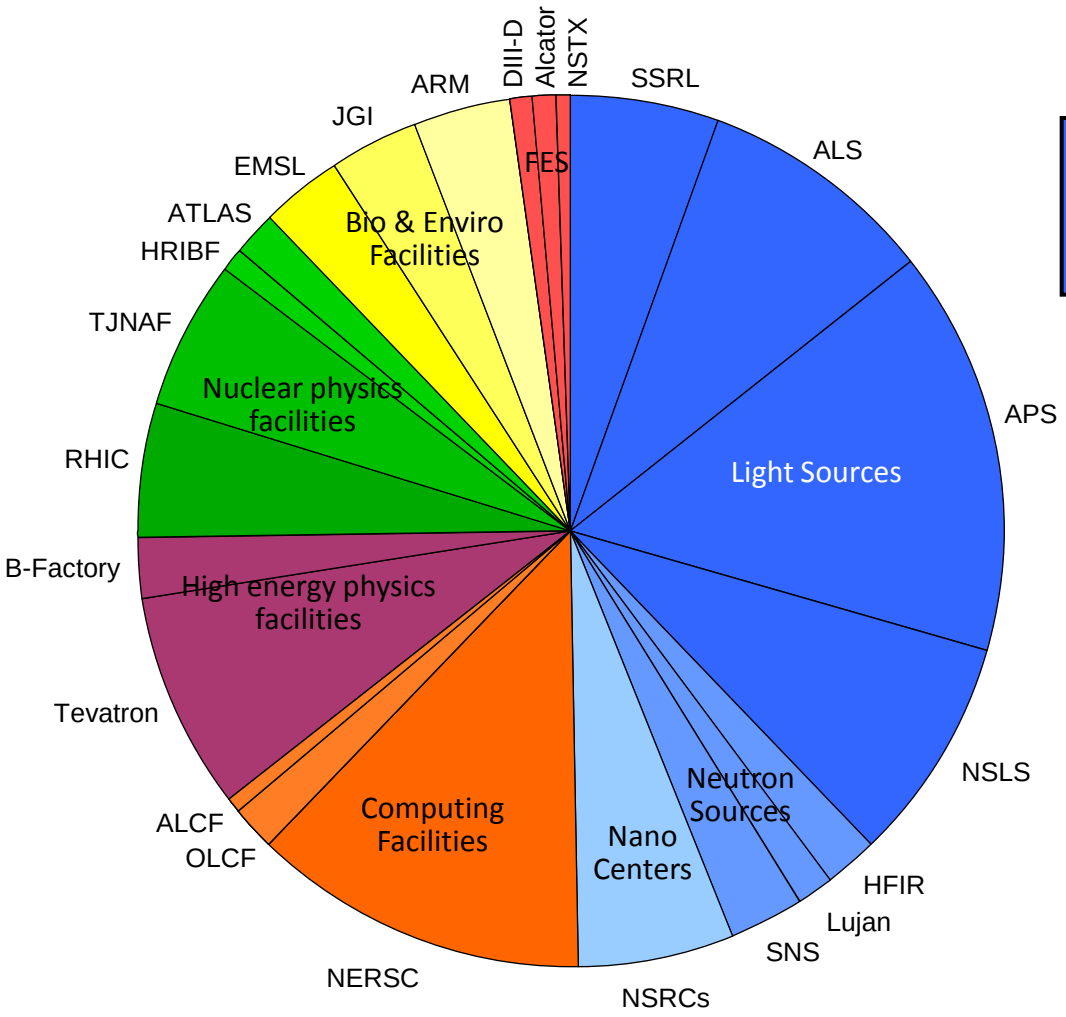
- Advanced **computational resources** – terascale to petascale computing and networks for open science
- Four **synchrotron light sources**, and two next-generation light sources in construction
- Three **neutron sources** for scattering
- **Particle accelerators/colliders/detectors** for high energy and nuclear physics
- **Fusion/plasma facilities**, including **ITER** which seeks to demonstrate a burning plasma
- Five **Nanoscale Science Research Centers** – capabilities for fabrication and characterization of materials at the nanoscale
- **Joint Genome Institute** for rapid whole genome sequencing
- **Environmental Molecular Science Laboratory** – experimental and computational resources for environmental molecular sciences
- **Atmospheric and Environmental Facilities** – capabilities for cloud and aerosol measurement and for carbon cycling measurements

# Distribution of Users by Facility

**~25,000 users at the facilities in FY 2010: ~1/2 from universities; ~1/3 from national labs; and the remainder from industry, other agencies, and international entities.**

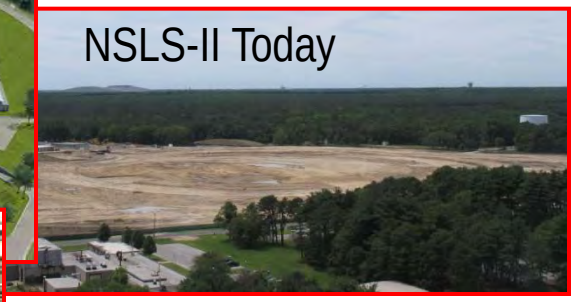
Breakdown by facility of ~25,000 users in FY 2010



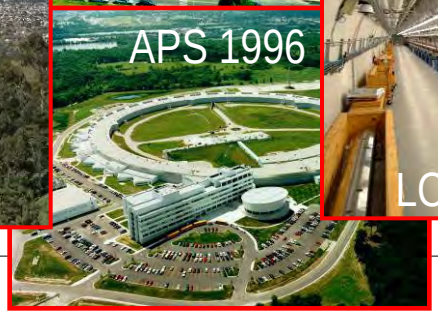

FY 2010 funding for the light sources is $258M, ~17% of the total funding for the operating facilities.

# 35 Years of Light Sources

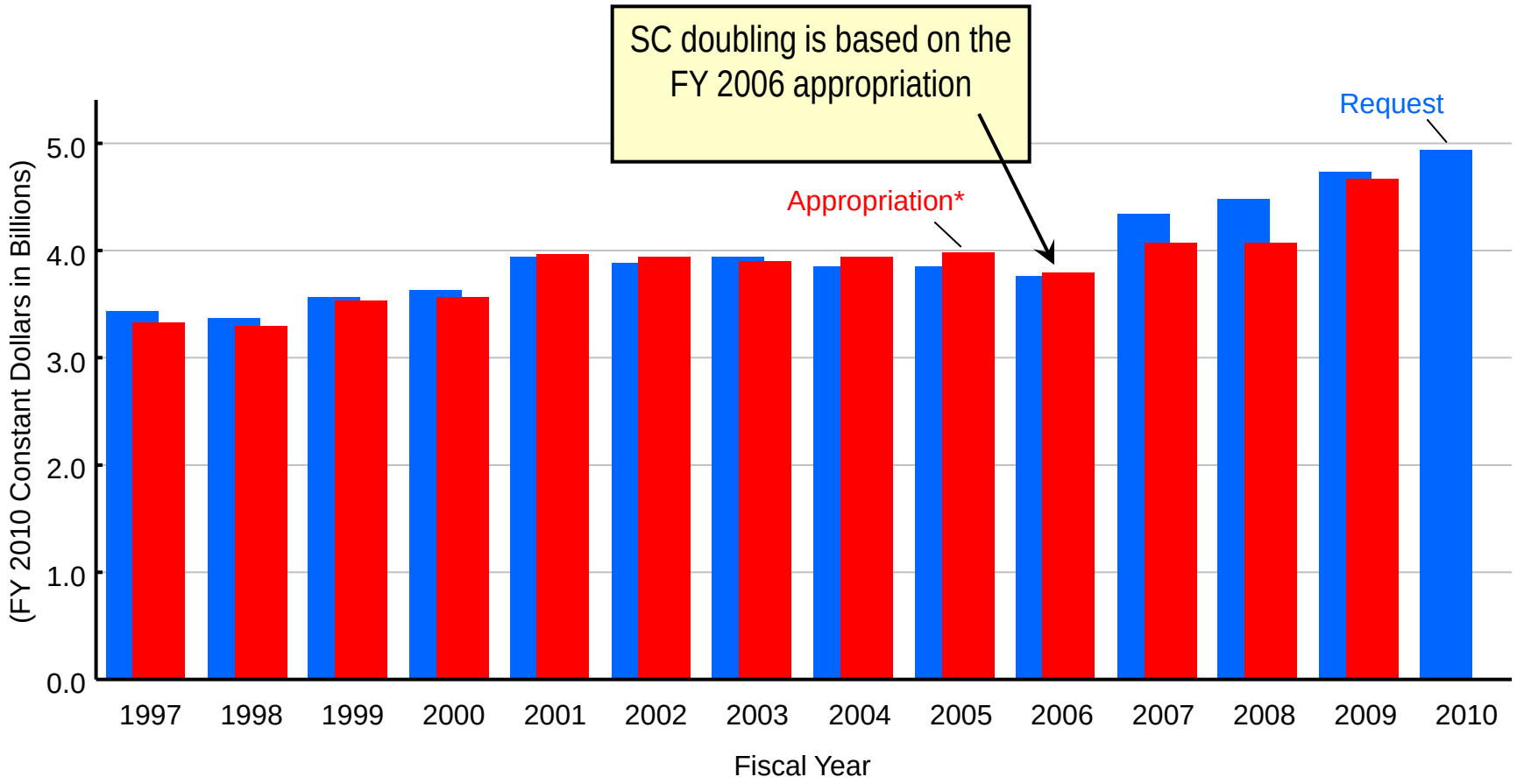







# SC Request vs. Appropriation (FY 2010 Constant $s)




* Appropriation amounts exclude Congressionally directed projects.

# Training the Next Generation of Scientists and Engineers

**The Department of Energy has >50 year history of training scientists, mathematicians, and engineers through research grants, the DOE national laboratories, and targeted education programs.**

- In FY 2008, more than 300,000 K-12 students; 21,000 educators; 3,000 graduate students; and 4,200 undergraduate students participated in opportunities at the DOE labs, funded by DOE and other federal and non-federal sources.
- SC will support over 4,400 graduate students and 2,700 post docs in FY 2009.
- In FY 2009, the Office of Workforce Development for Teachers and Scientists will support ~550 undergraduates in research internships at the DOE laboratories (and 1,175 in FY 2010 request) and ~280 K-16 educators.
- The DOE National Science Bowl attracts ~22,000 high school and middle school students every year.
- With ARRA funds and the FY 2010 request, SC initiated the DOE SC Graduate Fellowship Program, supporting over 160 graduate students in fields important to SC missions.
- SC proposes to increase the Graduate Fellowship Program to support approximately 400 graduate students in the out-years.

# Early Career Research Program

**The Department of Energy is now accepting proposals for the DOE Office of Science Early Career Research Program to support the research of outstanding scientists early in their careers.**

Purpose: To support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science.

# Status of FY 2010 Appropriations

## Office of Science
### FY 2010 Appropriations Status
(dollars in thousands)

| | FY 2009 | | FY 2010 | | |
|---|---|---|---|---|---|
| | Enacted Approp. | Recovery Act Approp. | Request to Congress | House Passed | Senate Mark |
| **Office of Science** | | | | | |
| Basic Energy Sciences | 1,571,972 | 555,406 | 1,685,500 | 1,675,000 | 1,653,500 |
| Advanced Scientific Computing Research | 368,820 | 161,795 | 409,000 | 409,000 | 399,000 |
| Biological & Environmental Research | 601,540 | 165,653 | 604,182 | 597,182 | 604,182 |
| High Energy Physics | 795,726 | 232,390 | 819,000 | 819,000 | 813,000 |
| Nuclear Physics | 512,080 | 154,800 | 552,000 | 536,455 | 540,000 |
| Fusion Energy Sciences | 402,550 | 91,023 | 421,000 | 441,000 | 416,000 |
| Science Laboratories Infrastructure | 145,380 | 198,114 | 133,600 | 133,600 | 133,600 |
| Science Program Direction | 186,695 | 5,600 | 213,722 | 190,932 | 194,722 |
| Workforce Development for Teachers & Scientists | 13,583 | 12,500 | 20,678 | 20,678 | 20,678 |
| Safeguards & Security | 80,603 | —— | 83,000 | 83,000 | 83,000 |
| Small Business Innovation Research/Tech. Transfer | —— | 18,719 | —— | —— | —— |
| Subtotal, Science | 4,678,949 | 1,596,000 | 4,941,682 | 4,905,847 | 4,857,682 |
| Advanced Research Projects Agency-Energy | 15,000 | —— | —— | —— | —— |
| Congressionally-directed projects | 93,687 | —— | —— | 37,740 | 41,150 |
| Subtotal, Science | 4,787,636 | 1,596,000 | 4,941,682 | 4,943,587 | 4,898,832 |
| Use of prior year balances | -15,000 | —— | —— | —— | —— |
| Less Advanced Research Projects Agency-Energy | -15,000 | —— | —— | —— | —— |
| Total, Office of Science | 4,757,636 | 1,596,000 [1/] | 4,941,682 | 4,943,587 | 4,898,832 |

[1/] $4,000 has been transferred to Departmental Administration for management and oversight.

# DOE Energy Innovation Hubs

***Proposed topics for Hubs:***

- **Solar Electricity (EERE)**
- **Fuels from Sunlight (SC)**
- **Batteries and Energy Storage (SC)**
- **Carbon Capture and Storage (FE)**
- **Electrical Grid Systems (OE)**
- **Energy Efficient Building Systems Design (EERE)**
- **Extreme Materials for Nuclear Fuel Cycles and Systems (NE)**
- **Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE)**

**Each Hub will comprise a world-class, multi-disciplinary and highly collaborative research and development team working largely under one roof. This team will focus on solving critical technology challenges that prevent large scale commercialization and deployment of the energy systems needed to address our Nation's greenhouse gas emission, energy security and workforce creation goals**

# Status of SC Recovery Act Projects

**The goals of the Recovery Act are articulated in the Act's "Statement of Purpose." Two that were key to our decisions are:**

- "To **preserve and create jobs** and promote economic recovery"; and
- "To provide investments needed to increase economic efficiency by **spurring technological advances in science** and health."

**SC ARRA projects were selected having specific characteristics:**

- Shovel-ready
- Enhance research infrastructure and support high-priority R&D
- Low risk (e.g., construction projects were baselined with in-place or imminent CD-3; research projects had proposals in hand or solicitations were to be fast)
- No out-year mortgages, with two exceptions (EFRCs and Graduate Fellowship/Early Career Awards)

# Status of SC Recovery Act Projects

## 51 projects totaling $1.6B

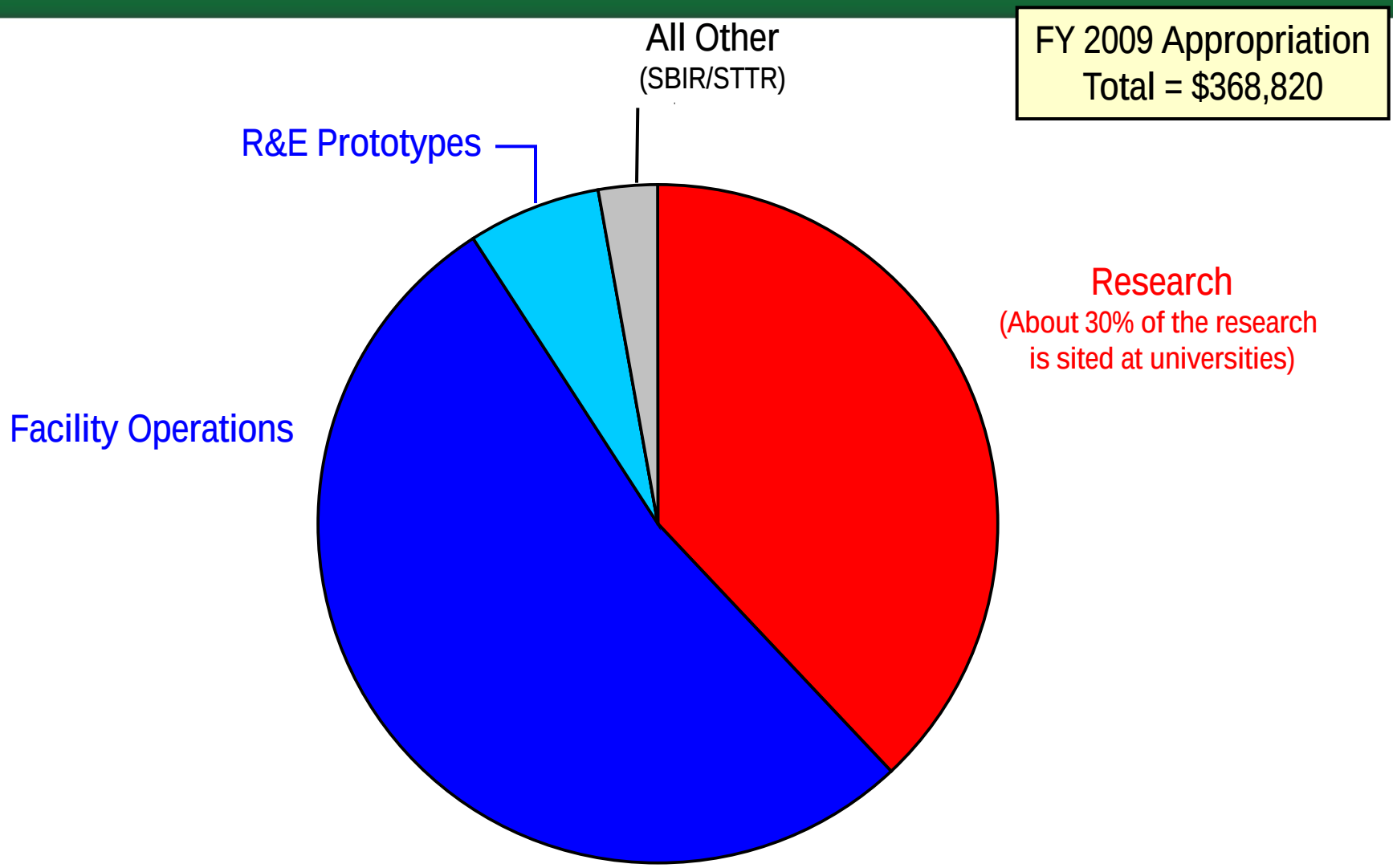
- **Acceleration of Ongoing Line-Item Construction Projects - $338.2M**
  - NSLS-II ($150.0M)
  - TJNAF 12 GeV upgrade ($65.0M)
  - Science Laboratory Infrastructure (SLI) Construction ($108.5M)
- **Acceleration of Major Items of Equipment - $171.1M**
  - NOvA MIE ($55.0M)
- **Upgrades to SC User Facilities - $391.0M**
  - Advanced Networking ($66.8M)
  - Atmospheric Radiation Measurement (ARM) Climate Research Facility ($60.0M)
  - Environmental Molecular Sciences Laboratory ($60.0M)
  - Light Source Instrumentation/Enhancements ($24.0M)
  - Nanoscale Science Research Center Instrumentation ($25.0M)
- **Laboratory General Plant Projects - $129.6M**
- **Scientific Research - $562.1M**
  - Energy Frontier Research Centers ($277.0M; forward-funded 5 years)
  - Energy Sciences Fellowships and Early Career Awards – ($97.5M; forward-funded 3-5 years)
- **Management and Oversight - $8.0M**

# Status of ASCR Recovery Act Projects

| | Amount |
|---|---|
| Advanced Networking Initiative | 66,818 |
| Magellan – Cloud computing for science | 32,768 |
| SciDAC-e – Bringing computational expertise to energy applications | 29,160 |
| Leadership Computing Upgrade | 19,900 |
| Advanced Computing Architectures | 5,179 |
| Total ASCR | **152,715** |

(dollars in thousands)

# ASCR FY2009 Support by Major Function



# ASCR Strategic Directions- 2010 & Beyond

## Science for Discovery – Discovering, developing, and deploying computational and networking tools for the analysis, modeling, simulation, and prediction of complex phenomena

- Develop mathematical descriptions, models, methods, and algorithms to further understanding of complex systems involving processes that span vastly different time and/or length scales
- Develop underlying understanding and software to enable scientists to make effective use of computers at extreme scales
- Advance key areas of computational science and discovery that advance the missions of the Office of Science through partnerships.

## National Scientific User Facilities – the 21st century tools of science

- Leadership Computing: **Over 1 billion processor hours were awarded through INCITE in 2009**

  The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) awardees have access to:
  - Argonne Leadership Computing Facility – 557 teraflop IBM Blue Gene/P, 80 terabytes of memory, and a 9.2 petabyte file system.
  - Oak Ridge Leadership Computing Facility – 1.64 petaflop Cray XT-5, 362 terabytes of memory, and a 10 petabyte file system.
- Production Computing for the Office of Science: **Over 3,100 users in 400 projects in 2009**

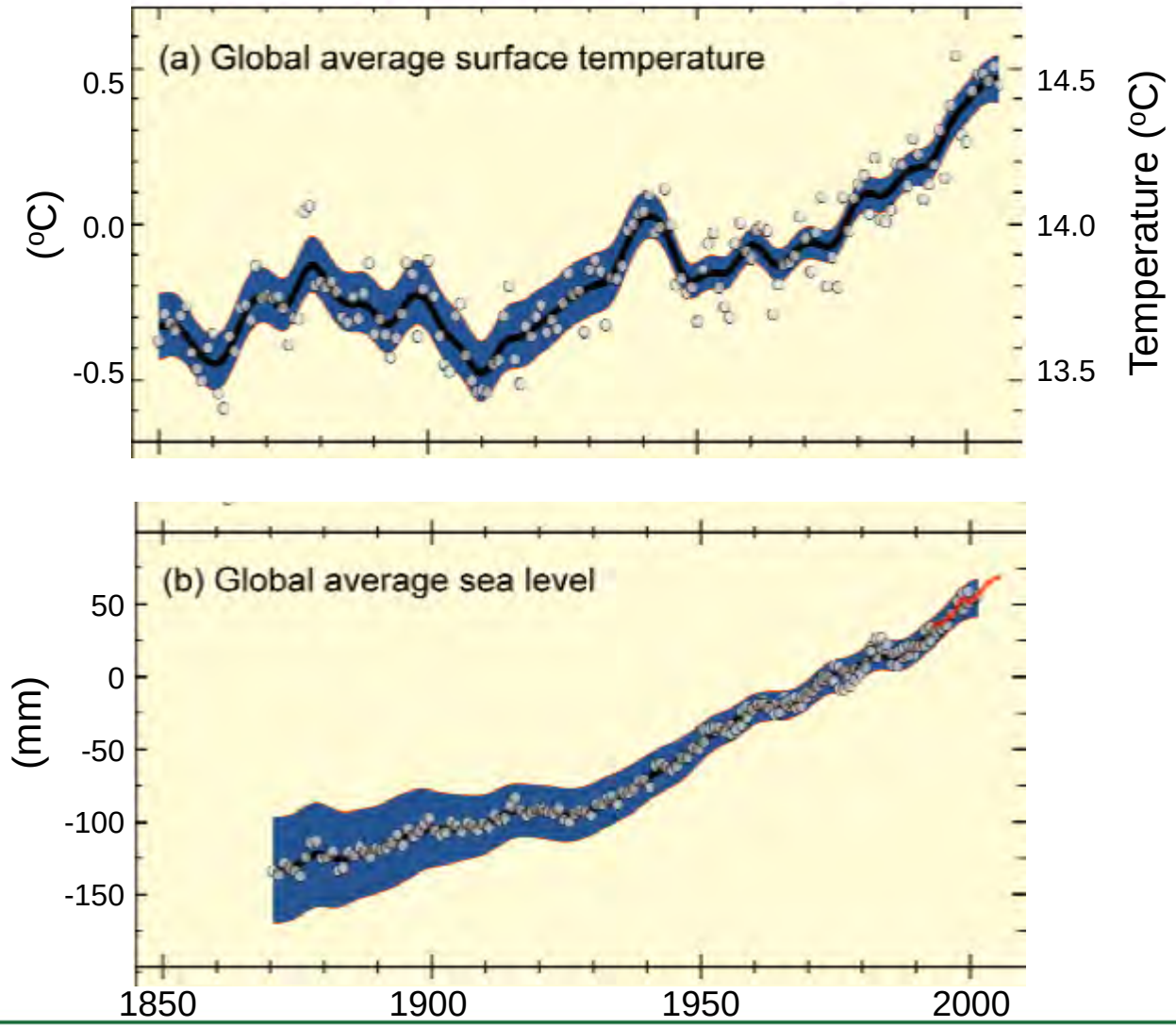
  Office of Science sponsored projects are served by:
  - National Energy Research Scientific Computing Center (NERSC) –
    - 355 teraflop Cray XT-5 with 78 terabytes of memory,
    - 6.7 teraflop IBM Power 5 with 3.55 terabytes of memory,
    - 3.1 teraflop Linux Opteron Cluster with 2.1 terabytes of memory
    - 59 petabyte shared file system.
- High Performance Scientific Network: **Thousands of scientists served worldwide**
  - The Energy Sciences network (ESnet) operates a 40Gbps network for open science data

# ASCR Strategic Directions- 2010 & Beyond

## Science for National Need – Delivering forefront scientific knowledge and state-of-the-art tools to serve the nation

- Many areas of research require leadership computing power for discovery
- Even with the newly harnessed petascale resources, many critical simulations are limited by computing power
- ASCR's strategic directions for 2010 and beyond continues to be:
  - Advance the state of the art in computational capability
  - Develop tools and methods for harnessing that capability
  - Bring this capability to bear on scientific questions with national need:
    - **Climate Modeling –** half of the runs for the U.S. contribution to the IPPC AR4 were done on ASCR computing systems; the Earth Systems Grid is the primary mechanism for sharing this data; and SciDAC supports the development of next generation codes
    - **Combustion –** advances in computing power move combustion simulations closer to real world conditions and provides new insights into how to improve fuel efficiency and reduce emissions
    - **Bioenergy –** working with DOE Bioenergy Research Centers, simulations of enzymes breaking down cellulose will help make cellulosic ethanol (energy from non-food crops) an economically viable option
    - **Nuclear Energy –** the worlds largest simulation of a reactor core was achieved at the ALCF and will help engineers to enhance safety and reduce waste in next generation reactors
    - **Fusion –** advances in computing power move fusion simulations closer to real world conditions and help engineers improve efficiency and design control systems
    - **Advanced Materials –** including the worlds first petascale application modeling superconductivity

# Recent Climate Trends



# Annual Greenhouse Gas Contributions