Update from the Office of Science

Advanced Scientific Computing Advisory committee
August 24, 2010

Dr. W. F. Brinkman
Director, Office of Science
U.S. Department of Energy

www.science.doe.gov
“When we fail to invest in research, we fail to invest in the future. Yet, since the peak of the space race in the 1960s, our national commitment to research and development has steadily fallen as a share of our national income. That’s why I set a goal of putting a full 3 percent of our Gross Domestic Product, our national income, into research and development, surpassing the commitment we made when President Kennedy challenged this nation to send a man to the moon.”

President Barack Obama
September 21, 2009

## Status of FY 2011 Budget Request and Appropriations

(dollars in thousands)

<table>
<thead>
<tr>
<th>Office of Science</th>
<th>FY 2010</th>
<th>Total Recovery Act</th>
<th>FY 2011 Request to Congress</th>
<th>House Mark</th>
<th>House Mark vs. Request</th>
<th>Senate Mark</th>
<th>Senate Mark vs. Request</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current Approp.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Advanced Scientific Computing Research</td>
<td>394,000</td>
<td>+161,795</td>
<td>426,000</td>
<td></td>
<td>418,000</td>
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<td>-1.9%</td>
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<tr>
<td>Basic Energy Sciences</td>
<td>1,636,500</td>
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<td>1,739,115</td>
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<tr>
<td>Biological &amp; Environmental Research</td>
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<td></td>
<td>614,500</td>
<td>-12,400</td>
<td>-2.0%</td>
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<tr>
<td>Fusion Energy Sciences</td>
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<td>380,000</td>
<td></td>
<td>384,000</td>
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<tr>
<td>High Energy Physics</td>
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<td>820,085</td>
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<tr>
<td>Nuclear Physics</td>
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<td>554,000</td>
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<td>-1.4%</td>
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<td>Workforce Development for Teachers &amp; Scientists</td>
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<td>Science Laboratories Infrastructure</td>
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<tr>
<td>Safeguards &amp; Security</td>
<td>83,000</td>
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<td>86,500</td>
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<tr>
<td>Science Program Direction</td>
<td>189,377</td>
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<td>214,437</td>
<td></td>
<td>208,000</td>
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<td>-3.0%</td>
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<tr>
<td>Small Business Innovation Research/Tech. Transfer (SC)</td>
<td>107,351</td>
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<td>——</td>
<td></td>
<td>——</td>
<td>——</td>
<td>——</td>
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<tr>
<td><strong>Subtotal, Science</strong></td>
<td>4,934,171</td>
<td>+1,596,000</td>
<td>5,121,437</td>
<td></td>
<td>4,881,650</td>
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<tr>
<td><strong>Earmarks</strong></td>
<td>76,890</td>
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<td>18,350</td>
<td></td>
<td>18,350</td>
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<tr>
<td><strong>Small Business Innovation Research/Tech. Transfer (DOE)</strong></td>
<td>60,176</td>
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<tr>
<td><strong>Total, Science</strong></td>
<td>5,071,237</td>
<td>+1,668,775</td>
<td>5,121,437</td>
<td></td>
<td>4,900,000</td>
<td>-221,437</td>
<td>-4.3%</td>
</tr>
</tbody>
</table>

ASCAC August 24, 2010
Office of Science – House Mark  
(dollars in Thousands)

<table>
<thead>
<tr>
<th></th>
<th>FY 2010 Approp.</th>
<th>FY 2011 Request</th>
<th>House</th>
<th>House vs. FY 2010 Approp.</th>
<th>House vs. Request</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC, Total</td>
<td>4,903,710</td>
<td>5,121,437</td>
<td>4,900,000</td>
<td>-3,710</td>
<td>-221,437</td>
</tr>
</tbody>
</table>

- No details are available, no vote on bill scheduled
- Includes $18,350 in Earmarks.
- Approximately the same as FY 2010.
- Ensures the United States’ continued global leadership of basic science research and develops the fundamental knowledge necessary for the next generation of energy innovations.
- Investments in HEP pushes the edges of scientific knowledge and fosters our nation’s world-leading scientists.
- Research in BES, FES, ASCR, NP, and BER build the foundation of knowledge that will enable us to transform our energy sector to be more secure and sustainable.
Office of Science – Senate Mark

(dollars in Thousands)

<table>
<thead>
<tr>
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<th>Senate</th>
<th>Senate vs. FY 2010 Approp.</th>
<th>Senate vs. Request</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC, Total</td>
<td>4,903,710</td>
<td>5,121,437</td>
<td>5,012,000</td>
<td>+108,290</td>
<td>+2.2%</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-109,437</td>
</tr>
</tbody>
</table>

- Includes $40.8M in Earmarks, $11M for Artificial Retina, $15.4M for Nuclear Medicine research, $100M to support EFRCs, $16M for Fuels from Sunlight Energy Innovation Hub, $22M for a new Batteries and Energy Storage Energy Innovation Hub, $35M for EPSCoR, and $5M for Graduate Fellowship.

- NP is down $8M from request but has the nuclear medicine added

- Funding increase in FY 2011 will support initiatives to advance scientific understanding for new energy technologies.

- Concerned about LHC’s planned shutdown; the Federal commitment to nuclear medicine research; cost increases and schedule delays related to the ITER project; and finding that the United States risks losing leadership and competitiveness in material science.
## Advanced Scientific Computing Research
(in whole dollars)

<table>
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<tr>
<th></th>
<th>House</th>
<th>Senate</th>
<th>Conference</th>
</tr>
</thead>
<tbody>
<tr>
<td>FY 2011 Request</td>
<td>$426,000,000</td>
<td>$426,000,000</td>
<td>$426,000,000</td>
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<tr>
<td>Committee Mark</td>
<td>424,800,000</td>
<td>418,000,000</td>
<td>—</td>
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<tr>
<td>Change to Request</td>
<td>-1,200,000</td>
<td>-8,000,000</td>
<td>—</td>
</tr>
</tbody>
</table>

Congressional Direction:

- **Mathematical, Computational, and Computer Sciences**
  - 424,800,000
  - —

  **Total Congressional Direction**
  - -1,200,000
  - —

Net unspecified program impact

- —
- -8,000,000

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*a/ The House subcommittee recommends $163,891,000 for Mathematical, Computational, and Computer Sciences Research, $1,200,000 below the request of $165,091,000.
$10 million is needed to FY 2011 to fund 150 additional fellowships

Purpose: To educate and train a skilled scientific and technical workforce in order to stay at the forefront of science and innovation and to meet our energy and environmental challenges and to couple the fellows into the Departments research

Eligibility:
- Candidates must be U.S. citizens and a senior undergraduate or first or second year graduate student to apply
- Candidates must be pursuing advanced degrees in areas of physics, chemistry, mathematics, biology, computational sciences, areas of climate and environmental sciences important to the Office of Science and DOE mission

Award Size:
- The three-year fellowship award, totaling $50,500 annually, provides support towards tuition, a stipend for living expenses, and support for expenses such as travel to conferences and to DOE user facilities.

FY 2010 Results:
- 150 awards were announced this summer using FY 2010 and American Recovery and Reinvestment Act funds.

FY 2011 Application Process:
- Funding Opportunity Announcement issued in Fall 2010
- Awards made in March 2011
Prospects for Solar Fuels Production

**What We Can Do Today**

$12/kg \text{H}_2 @ $3/pW PV
(BRN on SEU 2005)

**Two Limits**

- High capital costs
- Low capital costs

**Ultimate Goal**

solar microcatalytic energy conversion

---

Chemists do not yet know how to photoproduce \( \text{O}_2 \), \( \text{H}_2 \), reduce \( \text{CO}_2 \), or oxidize \( \text{H}_2\text{O} \) on the scale we need.

We do not know how to produce solar fuels in a cost effective manner.
Award of the “Fuel From Sunlight” Hub

- Winning team led by Cal Tech and LBNL
- Other institutions involved:
  - SLAC National Accelerator Laboratory
  - Stanford University
  - UC Berkeley
  - UC Santa Barbara
  - UC Irvine
  - UC San Diego
- Professor Nate Lewis leader
- Looking for a factor of 10 over nature
- Strong push to integrate processes to form a complete system
The Administration’s Energy Plan has two goals that require improvements in the science and technology of energy storage:

- Solar and wind providing over 25% of electricity consumed in the U.S. by 2025
- 1 million all-electric/plug-in hybrid vehicles on the road by 2015

- **Grid stability and distributed power require innovative energy storage devices**
  - Grid integration of intermittent energy sources such as wind and solar
  - Storage of large amounts of power
  - Delivery of significant power rapidly

- **Enabling widespread utilization of hybrid vehicles requires**:
  - Substantially higher energy and power densities
  - Lower costs
  - Faster recharge times

FY 2011 Energy Innovation Hub for Batteries and Energy Storage

Addressing science gaps for both grid and mobile energy storage applications

ASCAC August 24, 2010
World’s Most Powerful Computers for Open Science

Rankings from June, 2010 Top 500 Supercomputing List

#1 Jaguar

#9 ALCF

#17 ERSC
**Exascale Initiative**

**The Goal:** “Provide the United States with the next generation of extreme scale computing capability to solve problems of National importance in Energy, the Environment, National Security, and Science”

**Why do Exascale?**
- Environment
- Energy
- National Security
- Science and Innovation
- American Competitiveness

**Geologic sequestration**

**Massive Earth System Model ensembles**
(e.g. decadal forecasts, extreme weather)
Exascale Initiative Major Components

Platform R&D
2 Vendor Tracks
• Power
• Integration
• Risk Mitigation

Critical Technologies
(everyone benefits)
• Memory
• Nonvolatile storage
• Optics

Software and Environments
• Operating environment
• Systems Software
• System reliability
• Programming model

Co-design
• Physics Models
• Applied Math
• Performance models
• Simulators
• Applications integration with vendors

Platforms
• Early prototypes to ensure component integration and usefulness
• Risk mitigation for vendors – Non recoverable engineering cost

Exascale Initiative
Transitioning to Exascale
Applied Math and Computer Science

FY 2010: Focused on long lead time research for exascale:

- Applied Math
  - Complex mathematics with uncertainty quantification
    - Research that addresses the mathematical challenges involved in developing highly scalable approaches for uncertainty analysis in the modeling and simulation of complex natural and engineered systems.

- Computer Science
  - X-Stack Software Research
    - Emphasis on transformational computer science discoveries focused on the development of a scientific software stack that supports extreme scale scientific computing, from operating systems to development environments.
  - Advanced Architectures and Critical Technologies for Exascale Computing
    - Basic and applied research to address fundamental challenges in the design of energy-efficient, resilient hardware and software architectures and technology for high performance computing systems at exascale.
  - Scientific Data Management and Analysis at the Extreme
    - Innovative basic research in computer science for management and analysis of extreme-scale scientific data in the context of petascale computers and/or exascale computers with heterogeneous multi-core architectures.

Underpins Exascale
Linac Coherent Light Source or “LCLS” at SLAC
The World’s First X-ray Laser

LCLS uses 1/3 of linac

First X-rays:
~ 1 PM PDT 4/15/2009

Detection of X-ray at Far Hall ~ 1 PM PDT 4/22/2010

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Early Studies at LCLS: Nanocrystals in Water Microjet

**Spokesperson:** Henry Chapman et al.
collaboration of
Center for Free Electron Laser Science DESY
Arizona State University, Max Planck CFEL
ASG, SLAC, LLNL, CBST, Uppsala University

**John Spence** et al. ASU

**Liquid jet**

8 cm

**LCLS beam**

1.8 keV
60 - 300 fs pulses
$10^{13}$ photons / pulse

**x-rays:** 7 µm
**liquid jet:** 4 µm

**Front detector**

at 7 cm

**Back detector**

at 55 cm

ASCAC August 24, 2010
ITER (Latin for “the way”) is a first of a kind major international research collaboration on fusion energy.

U.S. is a 9.09% partner.

ITER Goals

- Designed to produce 500 MW of fusion power (Q > 10) for at least 300-500 seconds
- *Burning plasma* dynamics and control
  - U.S. emphasizes the value of ITER, its flexibility, and its diagnostics as a scientific instrument: develop a predictive capability of the burning plasma state
- Will optimize physics and integrate many of key technologies needed for future fusion power plants

Inertial Fusion Energy: Nearing Ignition

• The newly completed National Ignition Facility – the world’s most powerful laser system – recently began full operations
• NIF is on track to achieve the first laboratory demonstration of “ignition” or net energy gain
The U.S. is a critical and strategic partner in global scientific collaborations that push the boundaries of High Energy Physics. The U.S. has developed components for the Large Hadron Collider at CERN and hosts centers for data analysis.

At home, HEP builds on its investments in tools and facilities to capture the unique opportunities of neutrino science. These opportunities are fundamental to the science of particle physics.

At the heart of the DOE HEP program is the world’s most intense neutrino source at Fermilab, which serves MINERvA and MINOS and will support NOvA and the proposed LBNE (+$12,000K, HEP, initiated in FY 2011).
Progress Toward the Higgs Particle*

LEP Exclusion

Expected
Observed
±1σ Expected
±2σ Expected

Tevatron Exclusion

Tevatron Run II Preliminary, $L \leq 6.7 \text{ fb}^{-1}$

95% CL Limit/SM

$10$

$1$

100 110 120 130 140 150 160 170 180 190 200

$m_H (\text{GeV}/c^2)$

*D. Wright, LLNL, private communication

July 19, 2010

BESAC August 5, 2010
Accelerator Technology – Is it good enough?

- Long term waste storage needs dominated by actinides
- Fast Spectrum Reactors can burn actinides but require chemical processing
- Accelerator Driven Systems would allow the reduction of the actinides and burning of the spent fuel without chemical processing

Question is can accelerators be built with ~50MW of power in the beam and can associated targets be constructed
SBIR and STTR

• Continuous need for enhancing small businesses
• DOE-wide SBIR and STTR programs are managed by SC
• It is not a small program ~$150M/yr
• Steps are being taken to strengthen program

→ Moved up to report to Deputy Director in SC
→ Enhancing office to make it more effective
→ Strengthening involvement of DOE executive management

http://www.science.doe.gov/sbir/