Update from the Office of Science

Biological and Environmental Sciences
Advisory Committee
September 16, 2010

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

www.science.doe.gov
“We double the budget of key agencies, including the National Science Foundation, a primary source of funding for academic research, and the National Institute of Standards and Technology, which supports a wide range of pursuits – from improving health information technology to measuring carbon pollution, from testing “smart grid” designs to developing advanced manufacturing processes. And my budget doubles funding for the Department of Energy’s Office of Science which builds and operates accelerators, colliders, supercomputers, high-energy light sources, and facilities for making nano-materials. Because we know that a nation’s potential for scientific discovery is defined by the tools it makes available to its researchers.”

President Barack Obama
April 27, 2009
<table>
<thead>
<tr>
<th>Office of Science</th>
<th>FY 2010</th>
<th>FY 2011</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current</td>
<td>Total</td>
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<tr>
<td></td>
<td>Approp.</td>
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<tr>
<td>Use of PY Bal</td>
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<td><strong>Total, Science</strong></td>
<td>4,963,887</td>
<td>+1,669,248</td>
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## Biological and Environmental Research

(in whole dollars)

<table>
<thead>
<tr>
<th></th>
<th>House</th>
<th>Senate</th>
<th>Conference</th>
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<td>FY 2011 Request</td>
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<td>$626,900,000</td>
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<tr>
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<tr>
<td>Change to Request</td>
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<td>-12,400,000</td>
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</table>

Congressional Direction:

- Medical Applications
  - Change to Request: $7,000,000 b/ —

- Radiochemistry and Imaging Instrumentation
  - Change to Request: -15,400,000 c/ —

Total Congressional Direction: — -8,400,000 —

Net unspecified program impact: -13,283,000 -4,000,000 -626,900,000

### Recap of Biological and Environmental Research

#### Biological Systems Science

<table>
<thead>
<tr>
<th></th>
<th>House</th>
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<th>Conference</th>
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#### Climate and Environmental Sciences

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<thead>
<tr>
<th></th>
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<td>-8,000,000</td>
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</tbody>
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a/ The House subcommittee did not provide traditional language setting control level at BER.

b/ $11,000,000 is provided for artificial retina research. The Senate Committee encourages the Department to continue this research and meet its goal of producing a prosthesis with more than 1,000 electrodes, which would allow facial recognition, as quickly as possible.

c/ The funding request of $15,400,000 for nuclear medicine research efforts has been moved to Nuclear Physics to better address mission requirements.
$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 Department's 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 H_2 @ $3/pW PV
(BRN on SEU 2005)

High capital costs

Low capital costs

We do not know how to produce solar fuels in a cost effective manner.

Chemists do not yet know how to photoproduce O_2, H_2, reduce CO_2, or oxidize H_2O on the scale we need.

Ultimate Goal

solar microcatalytic energy conversion

Liquid fuel storage

Gas fuel storage

Compression

Liquid gas production

High capital costs

Low capital costs

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Chemists do not yet know how to photoproduce O_2, H_2, reduce CO_2, or oxidize H_2O on the scale we need.
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
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)
The Future: Exascale Computing and Climate Modeling

- Exascale computing will enable:
  - Simulation of clouds over their natural range of scales for global climate
  - Modeling fully turbulent exchange of heat and gases between the atmosphere and ocean
  - Robust climate models for early warning, adaptation, and mitigation
  - Higher resolution
Spatial resolution of climate models is increasing

- 300 km
- 150 km
- 75 km
- 25 km
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.
Linac Coherent Light Source or “LCLS” at SLAC
The World’s First X-ray Laser

LCLS uses 1/3 of linac

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

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

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

LCLS uses 1/3 of linac

electron beam

undulator hall
x-ray production

near hall
3 experiments

far hall
3 experiments

x-ray beam

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

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

First X-rays: ~ 1 PM PDT 4/15/2009
Early Studies at LCLS: Nanocrystals in Water Microjet

Spokesperson: \textbf{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

Spokesperson:

\textbf{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

8 cm

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

Liquid jet

LCLS beam

x-rays: 7 $\mu$m
liquid jet: 4 $\mu$m

front detector at 7 cm

back detector at 55 cm

BERAC September 16, 2010
• Identification of key lignin biosynthesis genes in switchgrass, providing potential targets for improving switchgrass as a bioenergy crop.

• Used synthetic biology toolkit to construct the first microbes to produce an advanced biofuel directly from biomass.

• Characterized soil microbial community structure to understand impacts of biomass crop growth on marginal lands.
• 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.
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).

The NuMI beamline provides the world’s most intense neutrino beam for the MINOS experiment and proposed NOvA and LBNE experiments.
Progress Toward the Higgs Particle*

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

95% CL Limit/SM

LEP Exclusion

Tevatron Exclusion

$\begin{align*}
\text{m}_H (\text{GeV/c}^2) \\
100 & 110 & 120 & 130 & 140 & 150 & 160 & 170 & 180 & 190 & 200 \\
1 & & & & & & & & & & \\
\end{align*}$

*Expected

Observed

$\pm 1\sigma$ Expected

$\pm 2\sigma$ Expected

SM=1

July 19, 2010

*D. Wright, LLNL, private communication
• 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
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/
What are the major knowledge gaps in climate models?

- Representation of **clouds** in climate models
- Direct and indirect effects of **aerosols** on climate
- Interactions of the **carbon cycle** and climate