



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# **FY 2011 Budget Request to Congress for DOE's Office of Science**

**Presented to the  
Advanced Scientific Computing  
Advisory Committee**

March 30, 2010

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# Office of Science (SC) FY 2011 Budget Request to Congress

(B/A in thousands)

	FY 2009		FY 2010	FY 2011		
	Current Base Approp.	Current Recovery Act	Current Approp.	Request to Congress	Request to Congress vs. FY 2010 Approp.	
Advanced Scientific Computing Research.....	358,772	161,795	394,000	426,000	+32,000	+8.1%
Basic Energy Sciences.....	1,535,765	555,406	1,636,500	1,835,000	+198,500	+12.1%
Biological & Environmental Research.....	585,176	165,653	604,182	626,900	+22,718	+3.8%
Fusion Energy Sciences.....	394,518	91,023	426,000	380,000	-46,000	-10.8%
High Energy Physics.....	775,868	232,390	810,483	829,000	+18,517	+2.3%
Nuclear Physics.....	500,307	154,800	535,000	562,000	+27,000	+5.0%
Workforce Development for Teachers & Scientists.....	13,583	12,500	20,678	35,600	+14,922	+72.2%
Science Laboratories Infrastructure.....	145,380	198,114	127,600	126,000	-1,600	-1.3%
Safeguards & Security.....	80,603	—	83,000	86,500	+3,500	+4.2%
Science Program Direction.....	186,695	5,600	189,377	214,437	+25,060	+13.2%
Small Business Innovation Research/Technology Transfer (SC).....	104,905	18,719	—	—	—	—
<b>Subtotal, Science.....</b>	<b>4,681,572</b>	<b>1,596,000</b>	<b>4,826,820</b>	<b>5,121,437</b>	<b>+294,617</b>	<b>+6.1%</b>
Congressionally-directed projects.....	91,064	—	76,890	—	-76,890	-100.0%
Small Business Innovation Research/ Technology Transfer (DOE).....	49,534	36,918	—	—	—	—
Use of prior year balances.....	-15,000	—	—	—	—	—
<b>Total, Office of Science.....</b>	<b>4,807,170</b>	<b>1,632,918</b>	<b>4,903,710</b>	<b>5,121,437</b>	<b>+217,727</b>	<b>+4.4%</b>



# SC Supports World-Leading, Open Access Scientific User Facilities

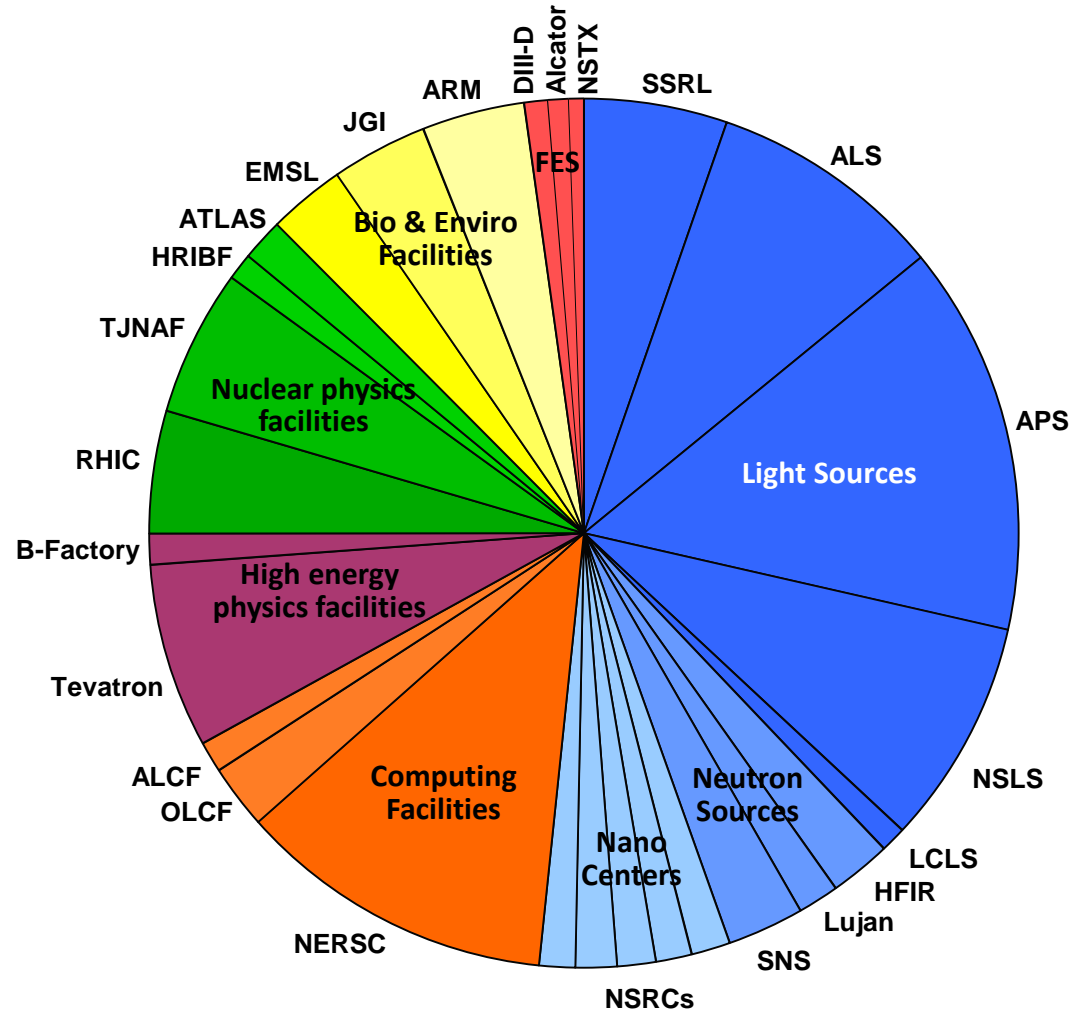
*User numbers continue to increase with more than 26,000 users expected in FY 2011*

Breakdown of the expected users in FY 2011 by facility.

Numbers of Users at SC Facilities

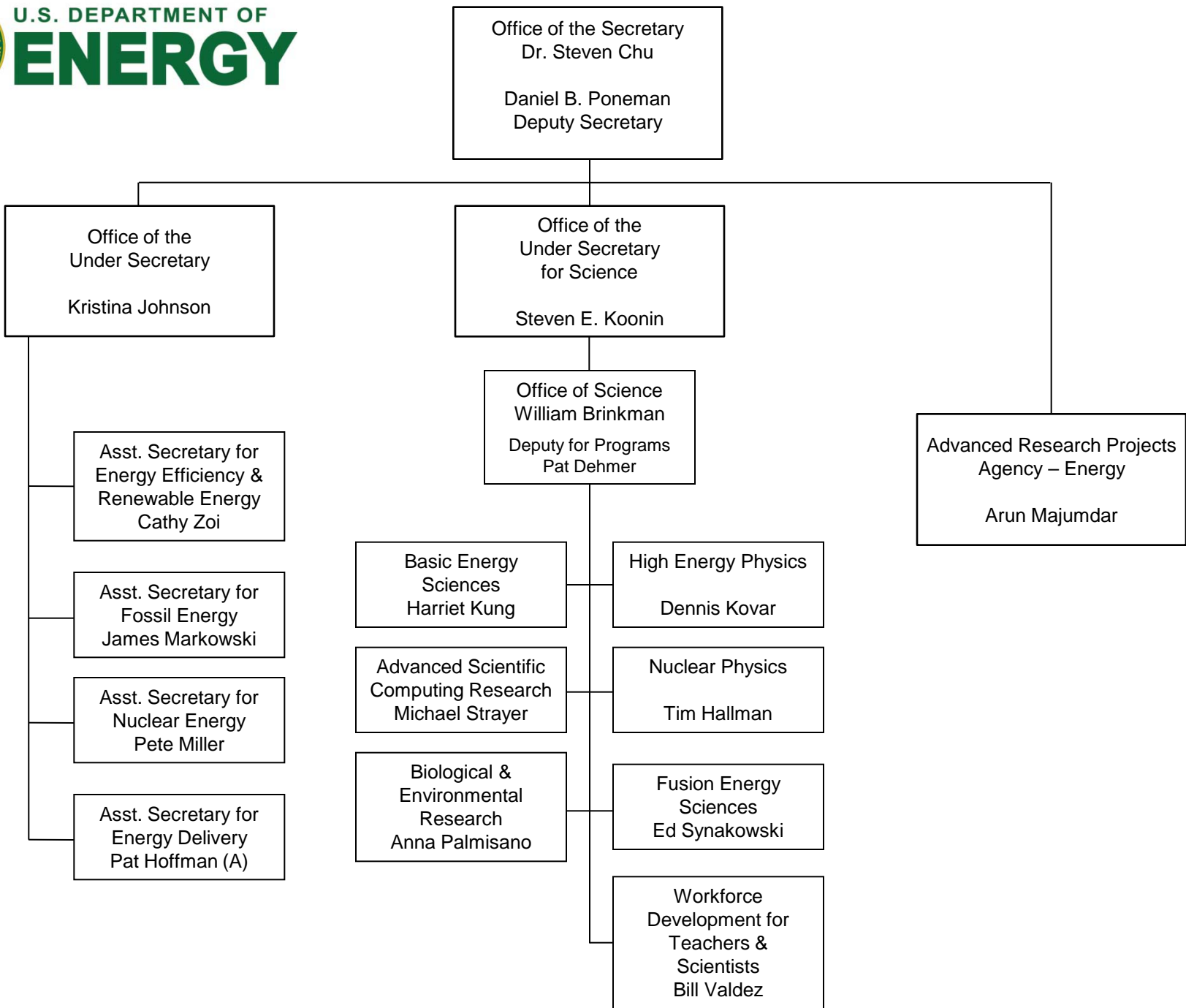
	FY 2009	FY 2010 (Est)	FY 2011 (Est)
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ASCR	3,696	3,850	4,025
BES	11,509	12,780	13,560
BER	2,716	2,690	2,690
FES	542	575	580
HEP	2,960	2,600	2,100
NP	3,170	3,260	3,300
<b>Total</b>	<b>24,593</b>	<b>25,755</b>	<b>26,255</b>





# U.S. DEPARTMENT OF ENERGY



# Office of Science FY 2011 Investment Highlights

**The FY 2011 budget advances discovery science and invests in science for national needs in energy, climate, and the environment; national scientific user facilities; and education and workforce development.**

## Discovery science addressing national priorities

- Energy Innovation Hub for Batteries and Energy Storage (+\$34,020K, BES)
- Enhanced activities in climate science and modeling (Regional and Global Climate Modeling, +\$6,495K; Earth System Modeling, +\$9,015K; Atmospheric System Research, +\$1,944K; ARM Climate Research Facility, +\$3,961K; BER)
- Individual investigator, small group, and Energy Frontier Research Centers (EFRCs) in areas complementing the initial suite of 46 EFRCs awarded in FY 2009 (+\$66,246K, BES)
- Leadership Computing Facilities operations and preparation for next generation of computer acquisitions for S&T modeling and simulation (\$34,832K, ASCR)
- Multiscale modeling of combustion and advanced engine systems (+\$20,000K, BES)

## Scientific user facilities—21<sup>st</sup> century tools of science, technology, and engineering

- Facility construction is fully funded; projects are meeting baselines
- 28 scientific user facilities will serve more than 26,000 users
- Several new projects and Major Items of Equipment are initiated (e.g., the Long Baseline Neutrino Experiment, +\$12,000K, HEP)

## Education and workforce development

- Expansions of the SC Graduate Fellowship Program (+\$10,000K, 170 new awards, WDTS) and the SC Early Career Research Program (+\$16,000K, 60 new awards, funded in all of the SC research programs)



# The Status of the DOE Energy Innovation Hubs

*Three new Hubs are launched in FY 2010 with SC leading the Fuels from Sunlight Hub*

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**Modeled after the Office of Science Bioenergy Research Centers, the Energy Innovation Hubs focus on critical energy technology challenges by building creative, highly-integrated research teams that can accomplish more, faster, than researchers working separately.**

**FY 2010 Hubs tackle three important energy challenges:**

- 1. Production of fuels directly from sunlight (SC)**
- 2. Energy-efficient building systems design (EERE)**
- 3. Modeling and simulation of advanced nuclear reactors (NE)**

**The Fuels from Sunlight Hub** will accelerate the development of a sustainable commercial process for the conversion of sunlight directly into energy-rich chemical fuels, likely mimicking photosynthesis, the method used by plants to convert sunlight, carbon dioxide, and water into sugar. In FY 2011, BES has budgeted \$24,300K for the 2<sup>nd</sup> year of the Fuels from Sunlight Hub. The FOA was released on 12/22/2009, and proposals are due on 3/29/2010.

To access the Fuels from Sunlight FOA (reference number DE-FOA-0000214) go to:

[https://www.fedconnect.net/FedConnect/PublicPages/PublicSearch/Public\\_Opportunities.aspx](https://www.fedconnect.net/FedConnect/PublicPages/PublicSearch/Public_Opportunities.aspx)

and search for "Fuels from Sunlight" in the search box (note that the search flag should be set to "Title" or "Title/Description").



# FY 2011 Energy Innovation Hub for Batteries and Energy Storage

*Addressing science gaps for both grid and mobile energy storage applications*

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**A new FY 2011 SC/BES Hub for Batteries and Energy Storage (\$34,020K) will address the critical research issues and will include:**

- **Design of advanced materials architectures:** design of low-cost materials that are self-healing, self-regulating, failure tolerant, and impurity tolerant
- **Control of charge transfer and transport:** control of electron transfer through designer molecules; electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity
- **Development of probes of the chemistry and physics of energy storage:** tools to probe interfaces and bulk phases with atomic spatial resolution and femtosecond time resolution
- **Development of multi-scale computational models:** computational tools to probe physical and chemical processes in storage devices from the molecular scale to system scale

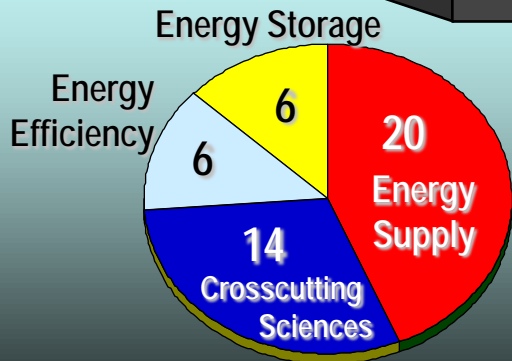
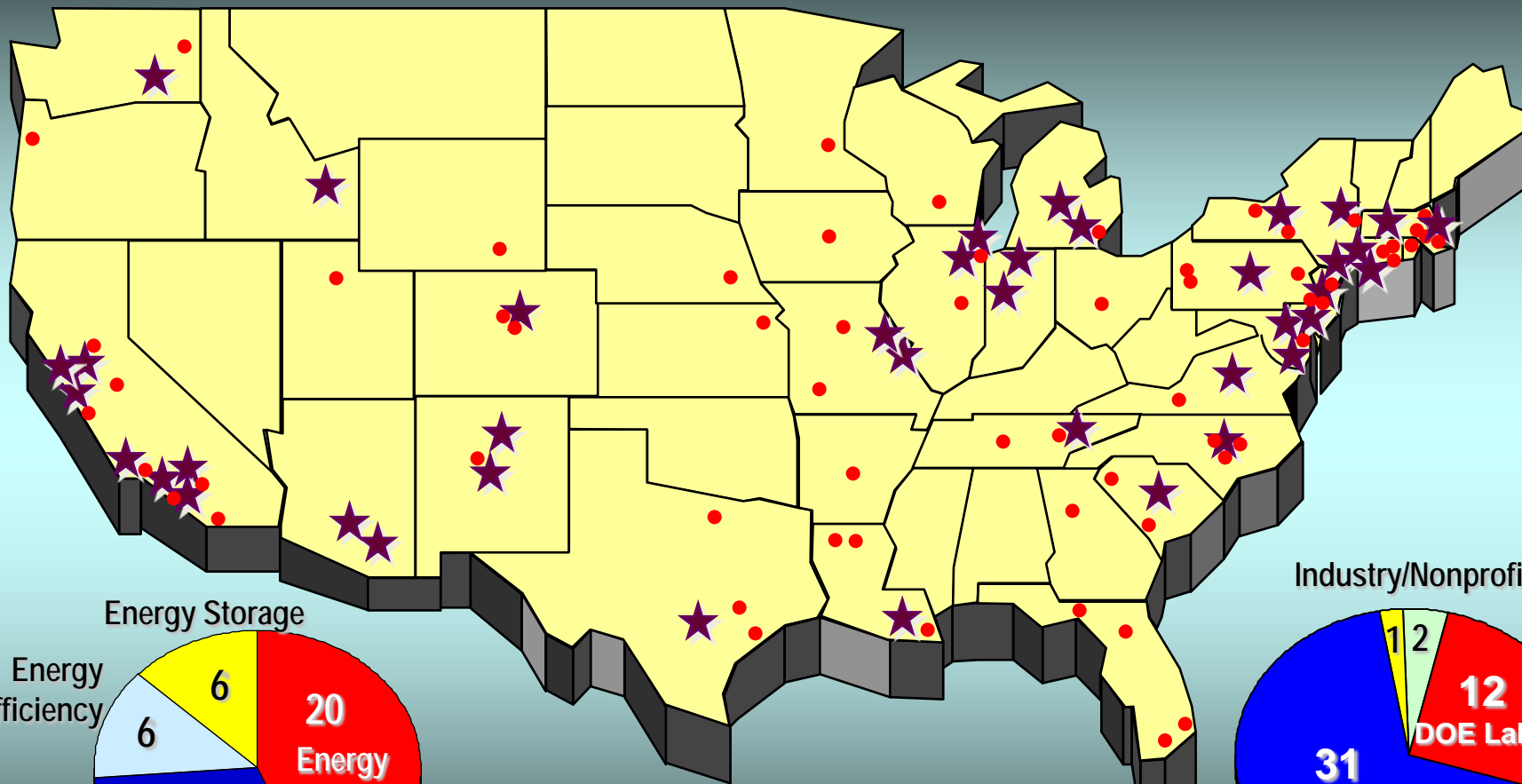


# The Status of the SC/BES Energy Frontier Research Centers

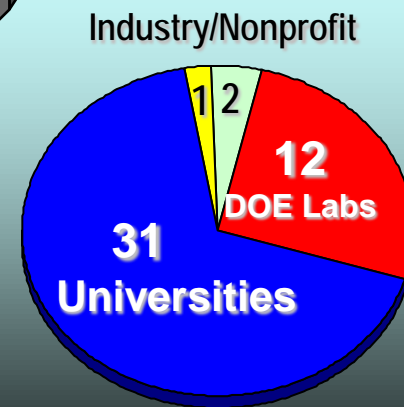
46 EFRCs were launched in late FY 2009 using FY 2009 Appropriations and Recovery Act Funds

46 centers awarded, representing 103 participating institutions in 36 states plus D.C

Energy Frontier Research Center Locations (★ Leads; ● Participants)



By Topical Category



By Lead Institution



# Leadership Computing Facilities

*The Office of Science leads the World in supercomputing capabilities*

**“Supercomputer modeling and simulation are changing the face of science and sharpening America’s competitive edge.”**

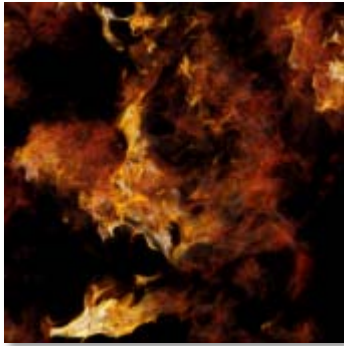
**Secretary Steven Chu**



**The Cray XT5 Supercomputer at Oak Ridge National Lab can perform over 2.3 quadrillion operations per second. It ranks #1 of the fastest computers world wide by Top500.org**

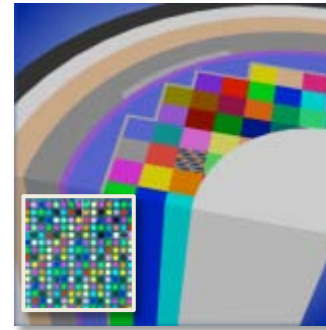


# Leadership Computing: Scientific Progress at the Petascale



## Turbulence

Understanding the statistical geometry of turbulent dispersion of pollutants in the environment.

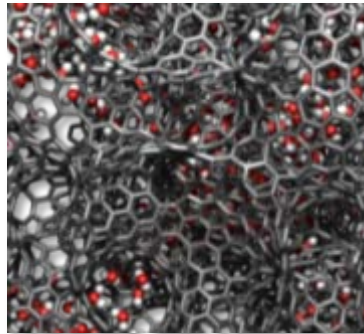


## Nuclear Energy

High-fidelity predictive simulation tools for the design of next-generation nuclear reactors to safely increase operating margins.

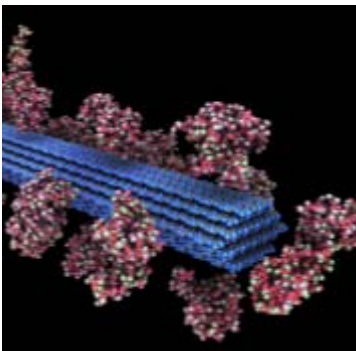
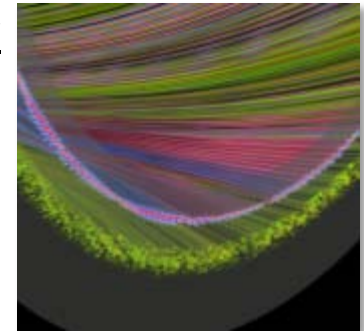
## Energy Storage

Understanding the storage and flow of energy in next-generation nanostructured carbon tube supercapacitors



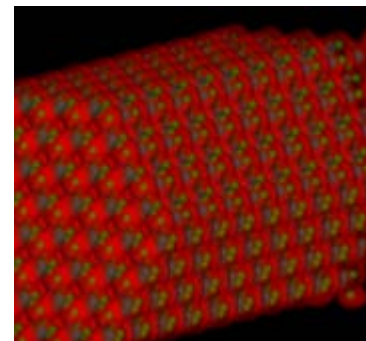
## Fusion Energy

Substantial progress in the understanding of anomalous electron energy loss in the National Spherical Torus Experiment (NSTX).



## Biofuels

A comprehensive simulation model of lignocellulosic biomass to understand the bottleneck to sustainable and economical ethanol production.



## Nano Science

Understanding the atomic and electronic properties of nanostructures in next-generation photovoltaic solar cell materials.



# Smart Truck Brands

Creation of Transformational Tractors, Trailers, and Components

*A coordinated program of engineering, fabrication, and testing that will be used to develop mechanical, aerodynamic, and engine improvements to fuel mileage of Class 8 Long Haul Trucks*



- 1.3 million Class 8 trucks in operation
- 300,000 new Class 8 trucks sold annually
- Average 6.7 MPG

*What will be the effects of a 3 mpg improvement from the Smart Truck Program?*

- Each truck will save approximately 4,300 gallons of fuel per year
- 95,000 lbs reduction of CO2 per truck per year
- Savings of approximately \$12,900 per truck per year in fuel costs (\$3/gallon diesel fuel)



# Aerodynamic Performance Testing Methods

## Jaguar CFD analysis of truck and mirrors

- Completed aerodynamic analysis of baseline truck in record time
- Completed aerodynamic design of initial aerodynamic add-on accessories to reduce the drag by 20%
- Reduced turn around time on CFD analysis to three hours from two days
- Established a rapid design schedule for new add-on parts (would not have been possible without the facilities and support that Oak Ridge provided)
- Verified Jaguar's CFD results with Straight Line Testing at Kennedy Space Center Shuttle Facility

***As a result of these accomplishments, the first set of add-on accessories/parts will be released this summer, providing fleets with substantial fuel mileage improvements.***



# Multi-scale Simulation of Internal Combustion Engines

*A new initiative to develop the science base for computational design of advanced engines*

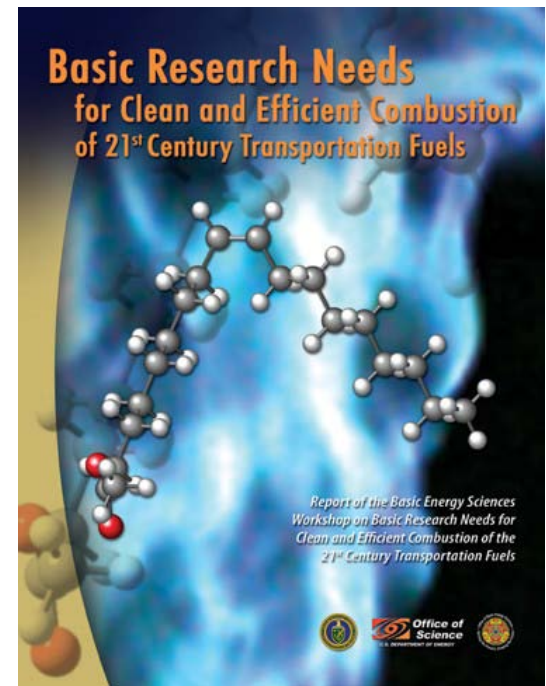
**Predictive simulation of combustion in an evolving fuel environment is essential for developing more efficient and cleaner engines.**

**The scientific community has provided a roadmap via:**

- BES workshop: *Basic Research Needs for Clean and Efficient Combustion*, October 2006
- ASCR/BES workshop: *Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale*, August 2009
- SC ongoing collaboration with EERE's Vehicle Technology Program

**The new BES activity (+\$20,000K) will provide:**

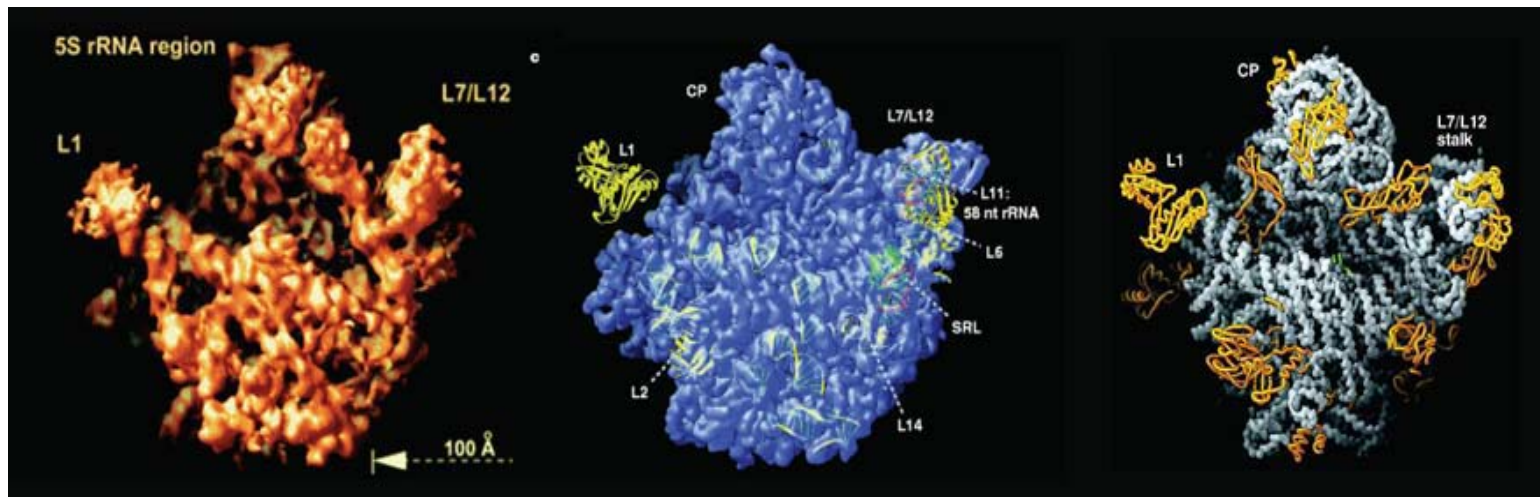
- **Models that span vast scale ranges:** coupling of combustion chemistry with turbulent flow requiring simulation over 9 orders of magnitude in space and time.
- **Improved understanding of fundamental physical and chemical properties:** multi-phase fluid dynamics, thermodynamic properties, heat transfer, and chemical reactivity.
- **Engine simulation:** science-based predictive simulation and modeling design



# The 2009 Nobel Prize Work Used all Four BES Light Sources

*Pls were supported by DOE/SC and NIH National Center for Research Resources*

- Ribosome translates the genetic instructions encoded by DNA into chains of amino acids that make up proteins. The ribosome is composed of two subunits: 30S, which reads the code; and 50S, which links up the amino acids.
- The structures of 30S and 50S have been crucial to understanding everything from how the ribosome achieves its amazing precision to how different antibiotics bind to the ribosome.
  - **Ramakrishnan** and **Steitz** used x-ray crystallography at the **NSLS** to gather structures of these two ribosome subunits: Ramakrishnan on 30S and Steitz on 50S.
  - **Steitz, Ramakrishnan,** and **Yonath** also performed studies at the **APS**. Most work was performed at the DOE beamline; Steitz and Yonath also used two other beamlines – GMCA-CAT and BIOCARS.
  - **Steitz** also performed work at the **ALS**.
  - **Yonath** also did early work at **SSRL** related to developing the cryo-cooling of ribosome particles.



The 50S subunit structure at 9Å resolution (left, 1998), 5Å resolution (middle, 1999), and 2.4Å resolution (right, 2000) (From Ban et al., 1998; 1999; 2000).





# Linac Coherent Light Source (LCLS) at SLAC

*Already producing new science today, the LCLS is the world's first x-ray free electron laser*

**LCLS is SC's newest x-ray light source user facility, providing an unprecedented combination of high spatial and temporal resolution for the investigation of atomic-scale structure and processes.**

**On target for an on time, within budget completion in FY 2010**

- Time between first start up and first light was, remarkably, under two hours!

**Meeting or exceeding design specifications to enable new science**

- Peak brightness 10 orders of magnitude greater than existing x-ray sources
- X-ray pulses as short as 2 millionths of a nanosecond (2 femtoseconds)

**Overwhelming demand for access**

- More than 850 researchers have applied for time on LCLS during the early access experimental runs, prior to CD-4



# Bioenergy Research Centers

*The BRCs have pioneered new approaches to accelerate biofuels research*

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\$75 million will support the fourth year of operations of the three BRCs

**Joint BioEnergy Institute (JBEI)**—research on model crops (*Arabidopsis* and rice) that can be transferred to bioenergy crops; lignin modification; synthetic biology approaches to fuels

- *Advanced biomass pretreatment using room temperature ionic liquids to remove lignin from plant cell walls improved biomass breakdown 5x.*
- *New cellulase enzyme more stable and active in ionic liquids at elevated temperatures and low pH.*

**Great Lakes Bioenergy Research Center (GLBRC)**—research on model plants and potential bioenergy plants; microbial biorefineries; sustainability of biofuel production

- *Improved screening of hydrolytic enzymes using gene expression approach coupled with enzyme screening and computational approaches – 100x more efficient than conventional methods*

**BioEnergy Science Center (BESC)**—research to overcome “recalcitrance” (resistance of plant fiber, or lignocellulose, to break down into sugars); gene discovery for recalcitrance; consolidated bioprocessing

- *New high throughput screening of chemical, structural, and genetic features of biomass – >100x faster than conventional methods.*
- *New imaging technologies to view cell wall at multiple scales to analyze recalcitrance*





# The Genomic Revolution

*Advances in DNA sequencing and analysis have revolutionized the study of biology*

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**Sequencing the 3 billion base-pair human genome took 13 years and multiple national and international partners. Today the DOE Joint Genome Institute sequences over a trillion base pairs annually.**

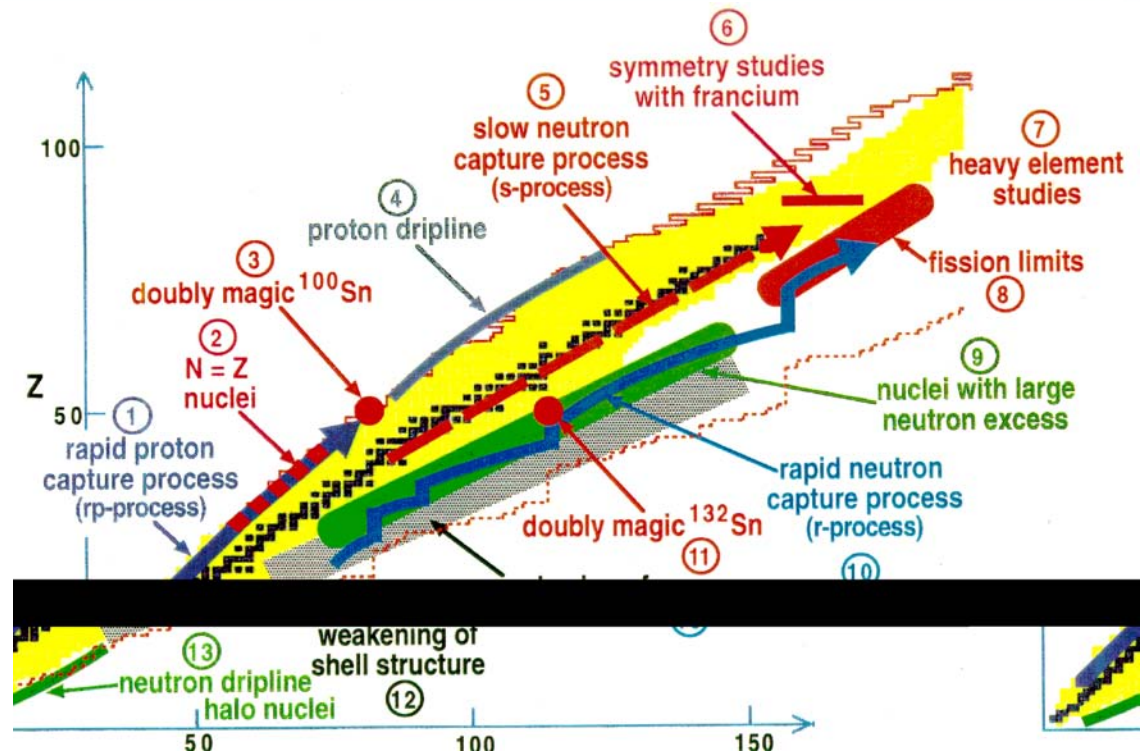
- DNA sequencing and analysis capabilities and the availability of genome data in the 1990s led to functional genomics, proteomics, metabolomics, systems biology, and synthetic biology.
- Genomic sequence information has dramatically increased our understanding of the biological processes of microbes and plants—knowledge that is being used to develop solutions for clean energy production, sequestration of atmospheric CO<sub>2</sub>, and remediation of contaminated environments.
- Recent accomplishments:
  - **Sequencing the 1.1 billion base-pair soybean genome**—The largest plant project sequenced at JGI and the largest plant sequenced by the whole genome shotgun strategy, the soybean sequence will accelerate crop improvements for energy production and environmentally sustainable food and feed production for agriculture.
  - **DOE JGI publishes the Genomic Encyclopedia of Bacteria and Archaea**—The initial 56 microbial genomes sequenced resulted in the discovery of tens of thousands of genes that provide insights into natural environmental processes and advance biotechnology.
  - **Viable microbes in toxic subsurface environments**—Genetic techniques demonstrate that microorganisms of the *Anaeromyxobacter* family, known to enzymatically reduce uranium to a less mobile form, can be detected in the most heavily contaminated environments and likely play a role in reducing the mobility of uranium in groundwater.



# The DOE Nuclear Physics Program

*Charting new directions at the frontiers of nuclear science*

The U.S. is a leader in studying the compelling questions of nuclear science, advancing our knowledge of the world, and leading to applications in energy research, medicine, national security, and isotopes for a wide variety of purposes.



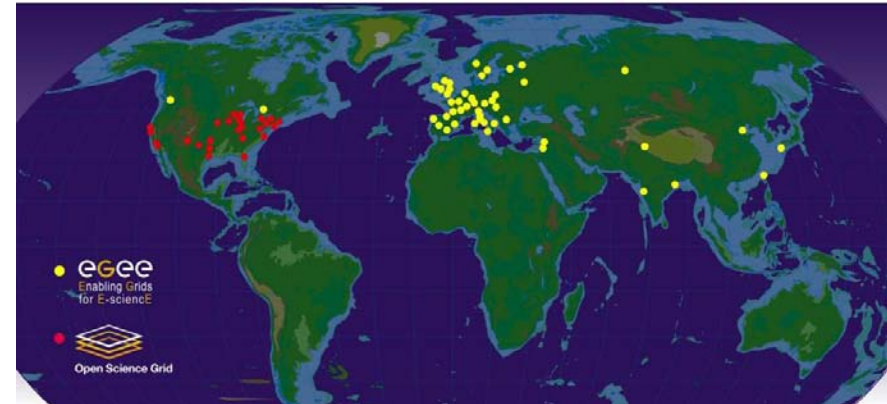
- **The Relativistic Heavy Ion Collider (RHIC)** is the only machine in the world colliding heavy ions at near light speed.
- **The Continuous Electron Beam Accelerator Facility (CEBAF)** is the world's most powerful probe for studying the nucleus of the atom.
- Investments in **Radioactive Ion Beam** experiments and capabilities (such as the **Facility for Rare Isotope Beams—FRIB**), probe the properties of rare nuclear isotopes to better understand the origin of the elements and fundamental symmetries of nature



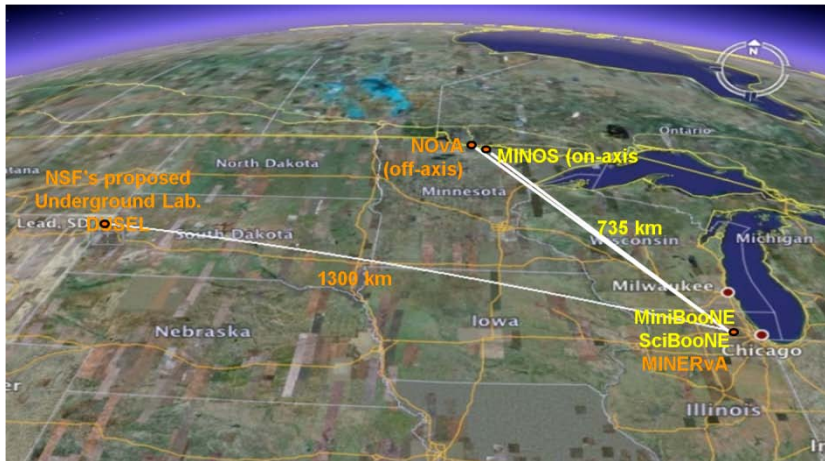
# The U.S. High Energy Physics Program

*Critical Investments in International Collaborations and World-Leading Domestic Facilities*

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.



Network sites of the Open Science Grid and Enabling Grids for E-science used for transmitting experimental data from the LHC to scientists worldwide.



The NuMI beamline provides the world's most intense neutrino beam for the MINOS experiment and proposed NOVA and LBNE experiments

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 (Critical Decision (CD) -0 for the LBNE was approved on January 8, 2010).**



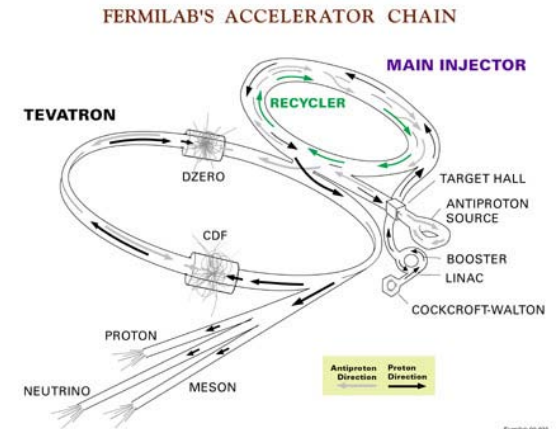
# Tevatron Accelerator Facility

*Continuing Tevatron operations through FY 2011 has the potential for big discoveries*

The Tevatron experiments systematically search for the Higgs Particle according to its potential mass.

With data collection through FY 2011, the Tevatron could rule out the existence of a Standard Model Higgs Particle.

The Tevatron has superior sensitivity to the Standard Model Higgs than the LHC at CERN.



## Search for the Higgs Particle

Status as of March 2009





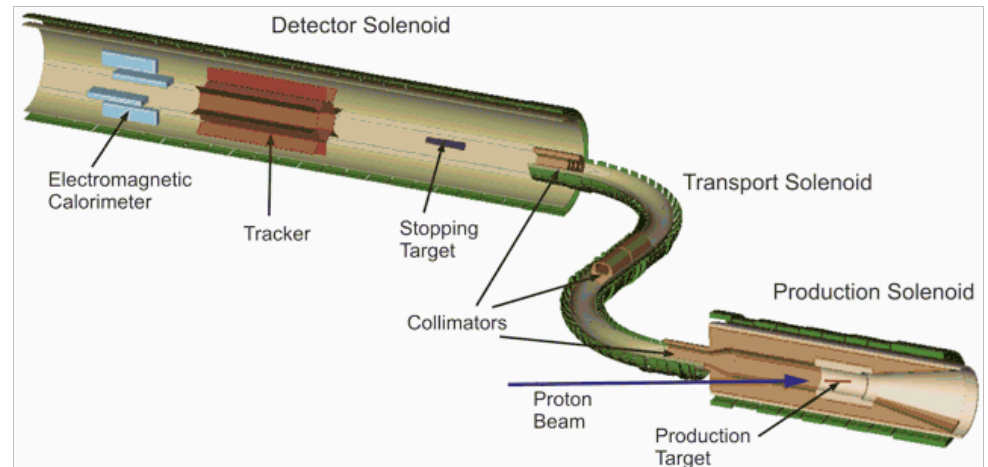
# The U.S. High Energy Physics Program

*The U.S. is uniquely positioned for a world-leading program at the Intensity Frontier*



- CD-0 for LBNE was approved in Jan, 2010
- FY 2011 Budget Request provides for PED

- CD-0 for Mu2e was approved in Nov, 2009
- FY 2011 Budget Request provides for PED



# Office of Science Early Career Research Program

*Investment in FY 2011 will bring 62 new scientists into the program*

**\$16 million will be available in FY 2011 to fund about 60 additional Early Career Research Program awards at universities and DOE national laboratories.**

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

**Eligibility:** Within 10 years of receiving a Ph.D., either untenured academic assistant professors on the tenure track or full-time DOE national lab employees

**Award Size:**

- University grants \$150,000 per year for 5 years to cover summer salary and expenses
- National lab awards \$500,000 per year for five years to cover full salary and expenses

**FY 2010 Results:**

- 69 awards funded via the American Recovery and Reinvestment Act
- 1,750 proposals peer reviewed to select the awardees
- 47 university grants and 22 DOE national laboratory awards
- Awardees are from 44 separate institutions in 20 states

**FY 2011 Application Process:**

- Funding Opportunity Announcement issued in Spring 2010
- Awards made in the Second Quarter of 2011

[http://www.science.doe.gov/SC-2/early\\_career.htm](http://www.science.doe.gov/SC-2/early_career.htm)



# DOE Office of Science Graduate Fellowships

*The FY 2011 request doubles the number of graduate fellowships in basic science*

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## **\$10 million will be available in FY 2011 to fund about 170 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

### **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:**

- 160 awards will be made this Spring with 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

