



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Office of Science Update

APS March Meeting
March 17, 2016

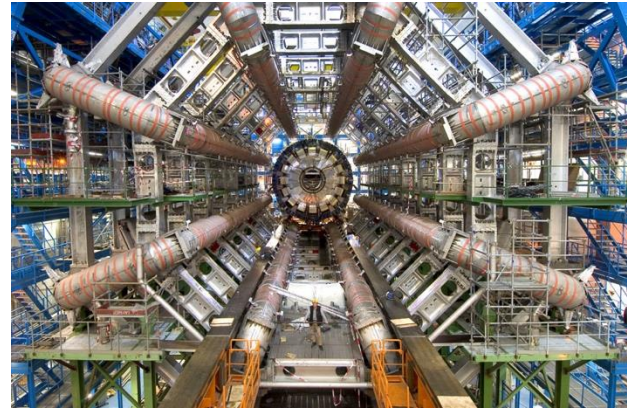
Cherry A. Murray
Director, Office of Science
cherry.murray@science.energy.gov

Department of Energy Mission Areas

Energy



Science



Nuclear Safety and Security

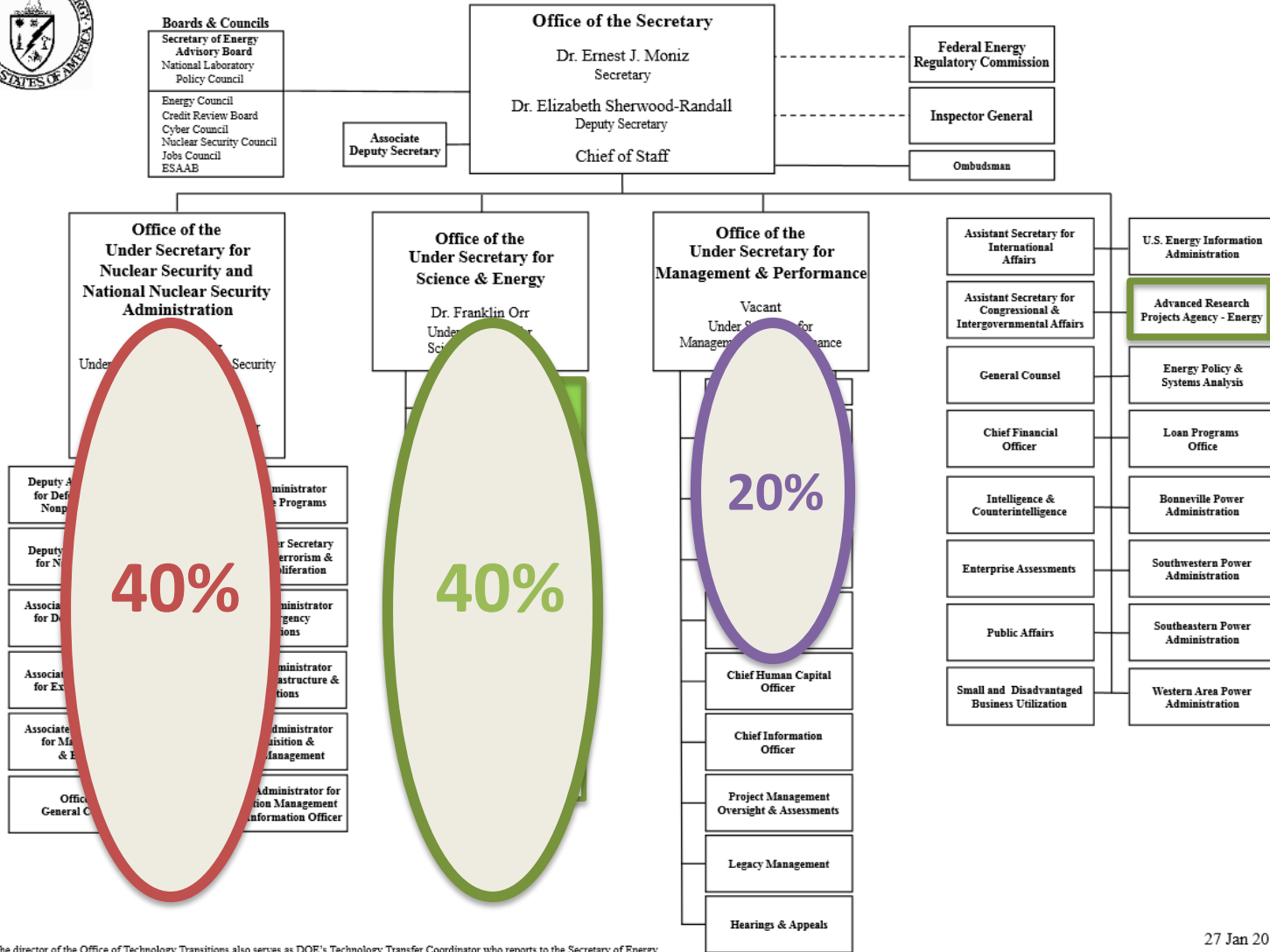


Environmental Cleanup



DOE Organization Chart 2016

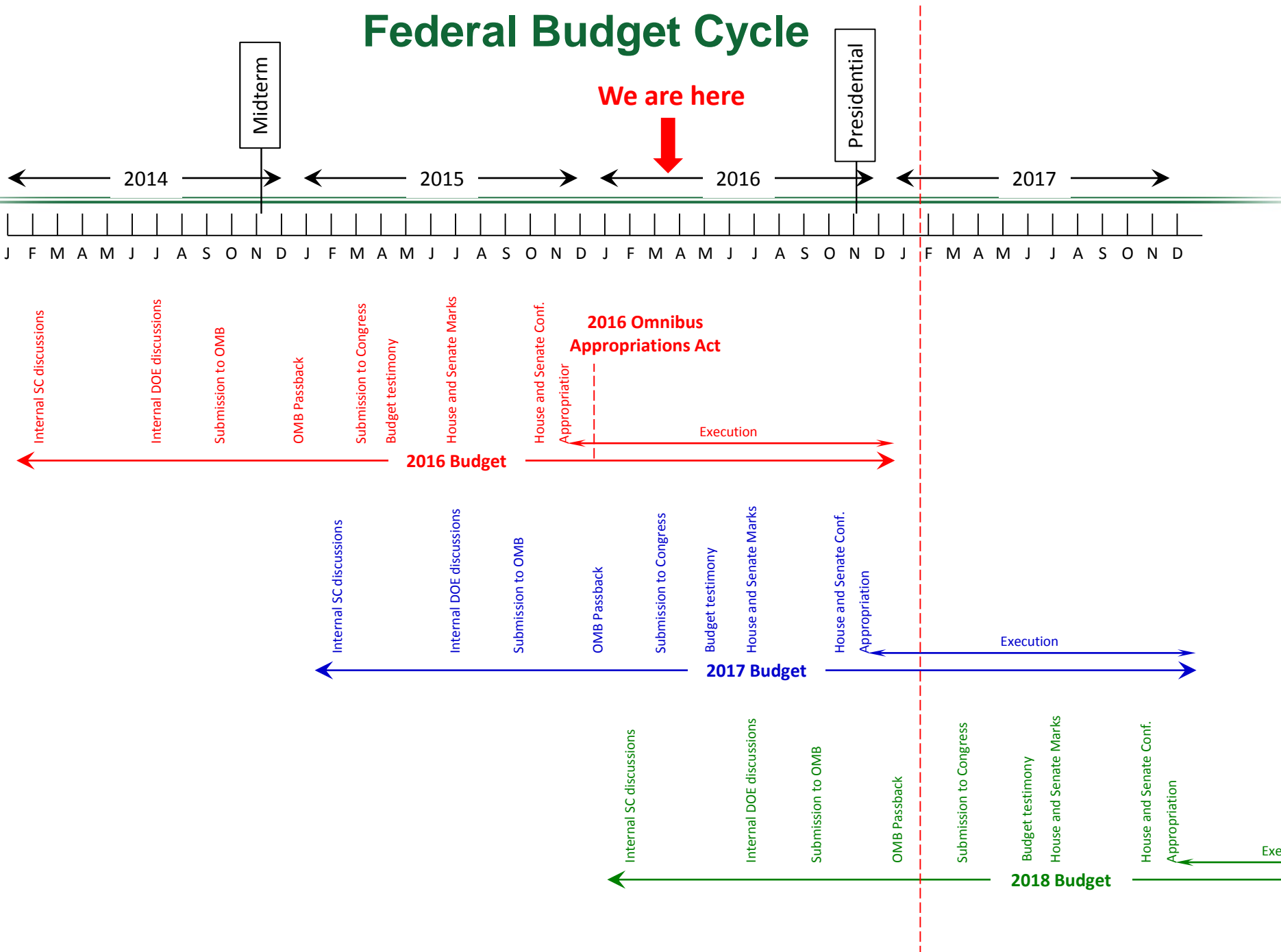
DEPARTMENT OF ENERGY



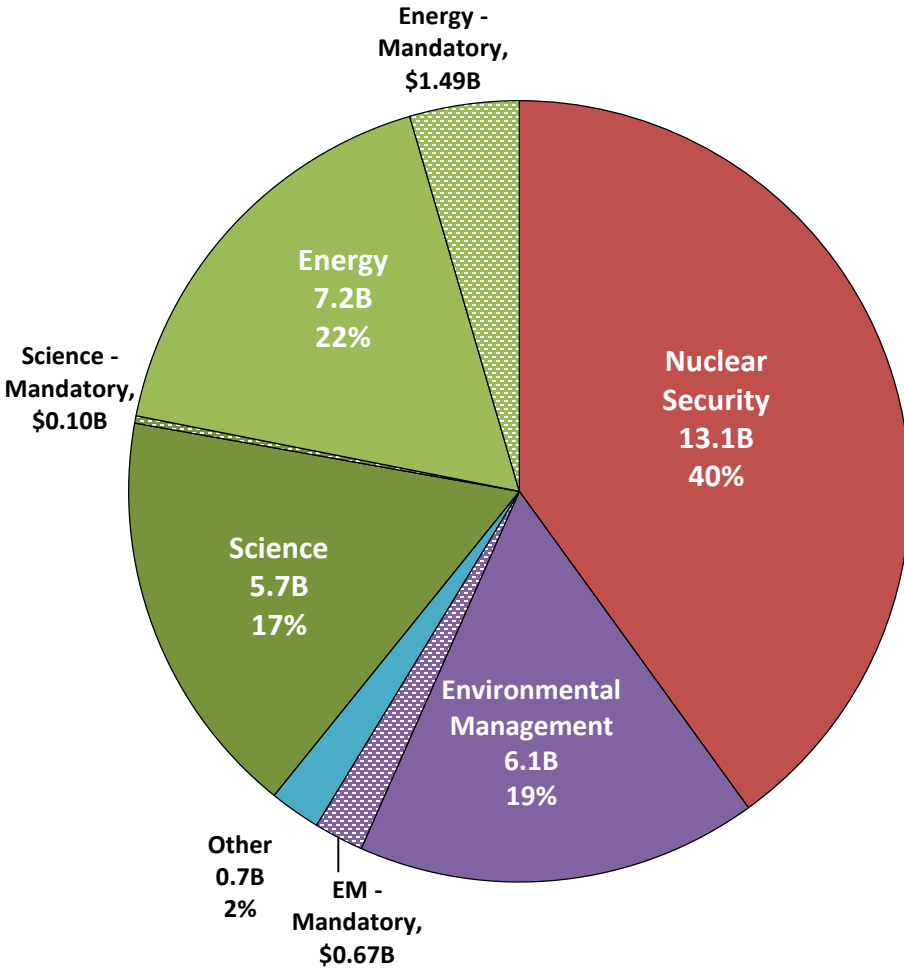
¹ The director of the Office of Technology Transitions also serves as DOE's Technology Transfer Coordinator who reports to the Secretary of Energy

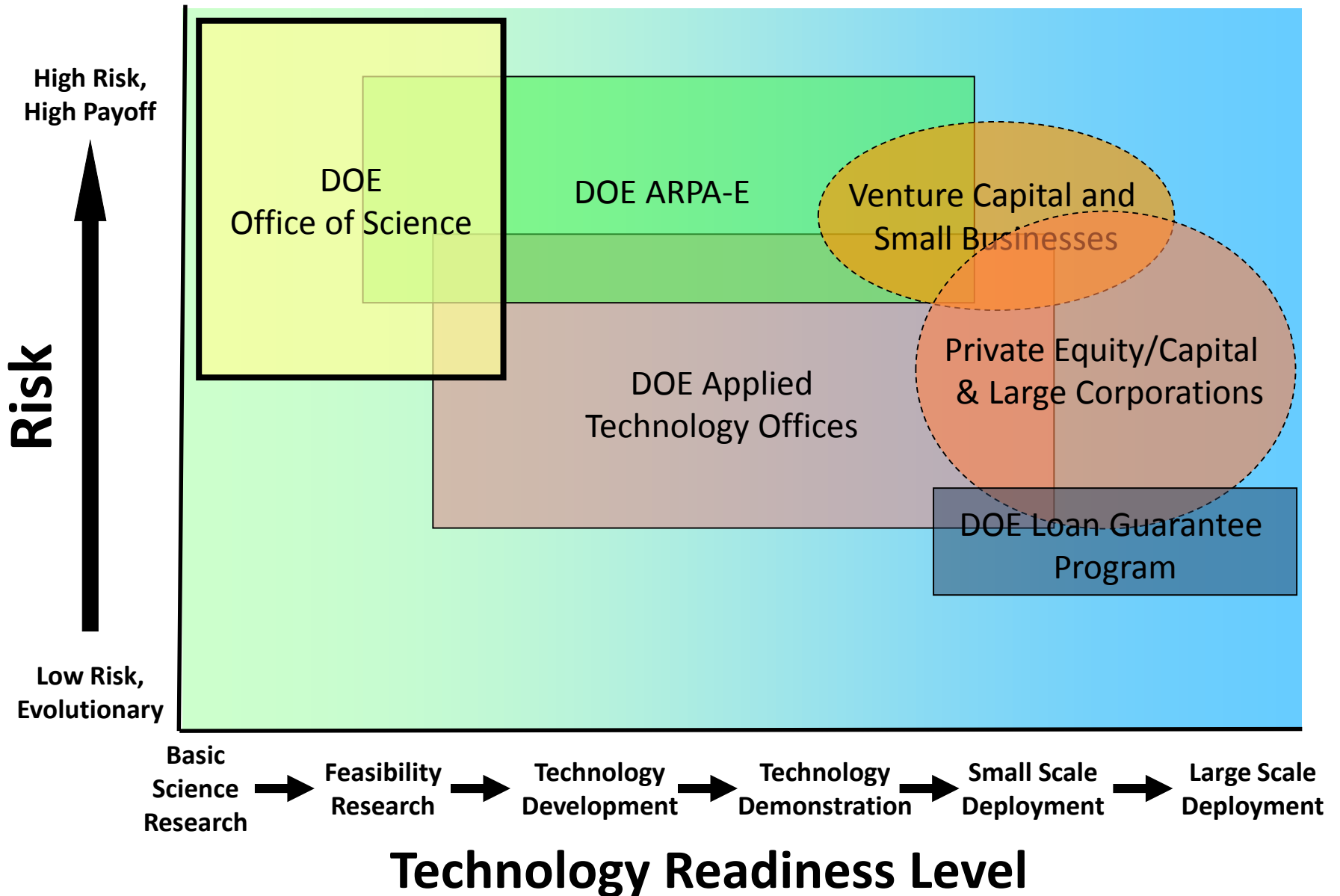
27 Jan 2016

Federal Budget Cycle

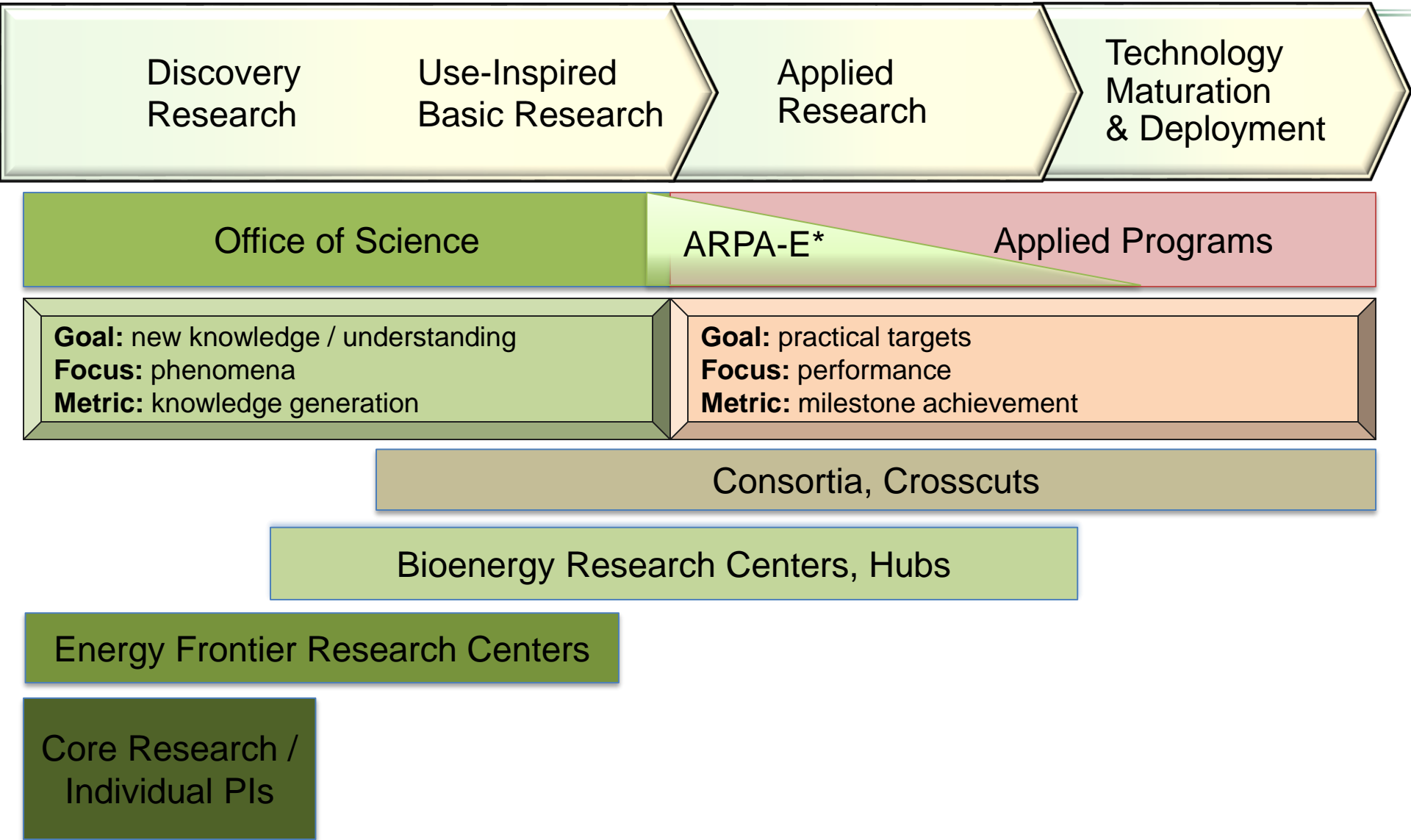


President's DOE FY 2017 Proposed Budget





DOE Funding Modalities



Discovery Research

Use-Inspired Basic Research

Applied Research

Technology Maturation & Deployment

Office of Science

ARPA-E*

Applied Programs

Goal: new knowledge / understanding
Focus: phenomena
Metric: knowledge generation

Goal: practical targets
Focus: performance
Metric: milestone achievement

Consortia, Crosscuts

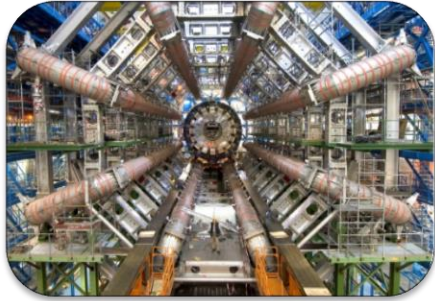
Bioenergy Research Centers, Hubs

Energy Frontier Research Centers

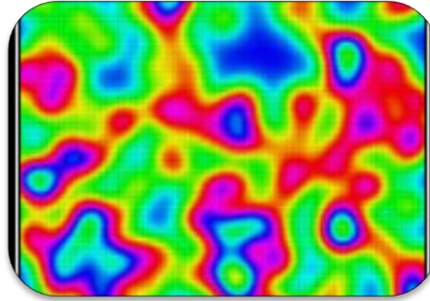
Core Research / Individual PIs



Office of Science FY16 - \$5.35B



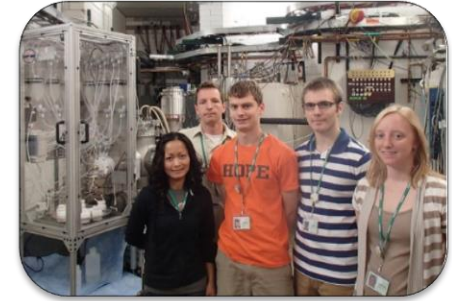
Largest Supporter of Physical Sciences in the U.S.*



Research: 42%, \$2.2B



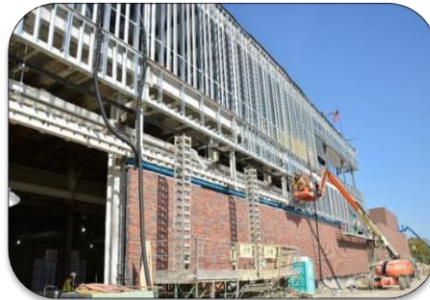
~40% of Research to Universities



> 20,000 Scientists Supported



Funding at >300 Institutions including all 17 DOE Labs



Construction: 13.5%, \$723M



Facility Operations: 38%, \$2.02B



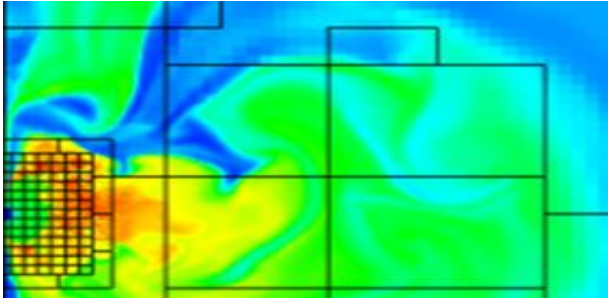
>30,000 Scientific Facility Users**

* 43% of all physical sciences, 30% of computer science and math

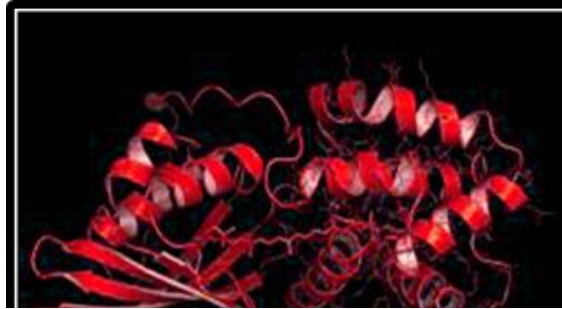
** from all 50 states and DC



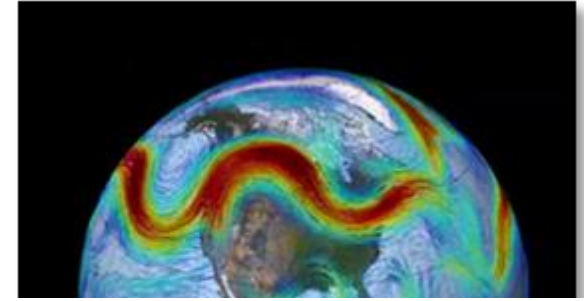
Office of Science Programs



**Advanced Scientific Computing
Research**
FY2016 \$621M



Basic Energy Sciences
FY2016 \$1849M



**Biological and Environmental
Research**
FY2016 \$609M

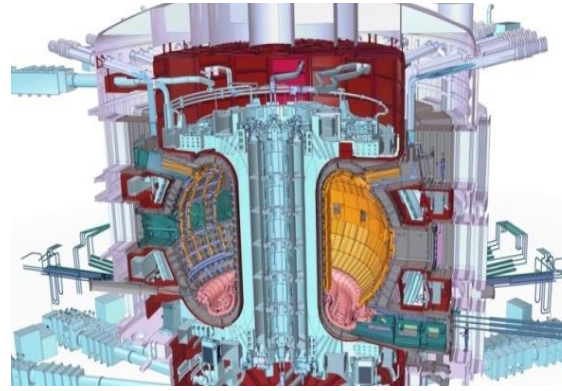
High Energy Physics

FY2016 \$795M



Fusion Energy Sciences

FY2016 \$438M



Nuclear Physics

FY2016 \$617M



U.S. DEPARTMENT OF
ENERGY

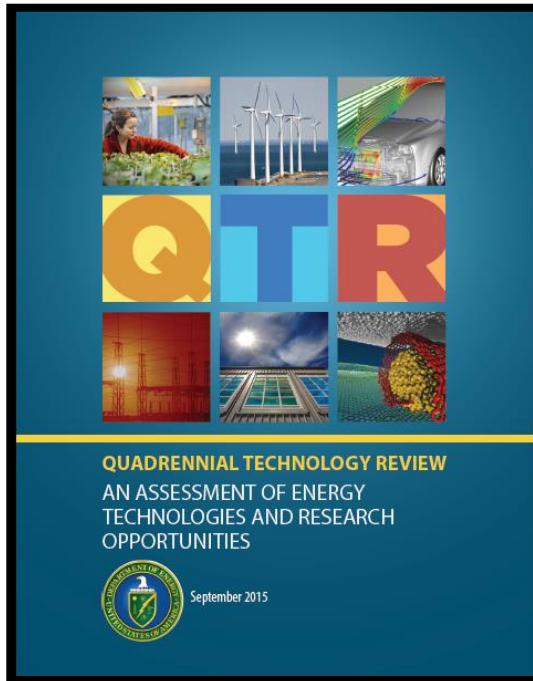
Office of
Science

Office of Science Workshops

We use workshops, such as the Basic Research Needs Workshops in BES, Federal Advisory Committee Reports and National Academies Studies to engage the scientific community in planning.



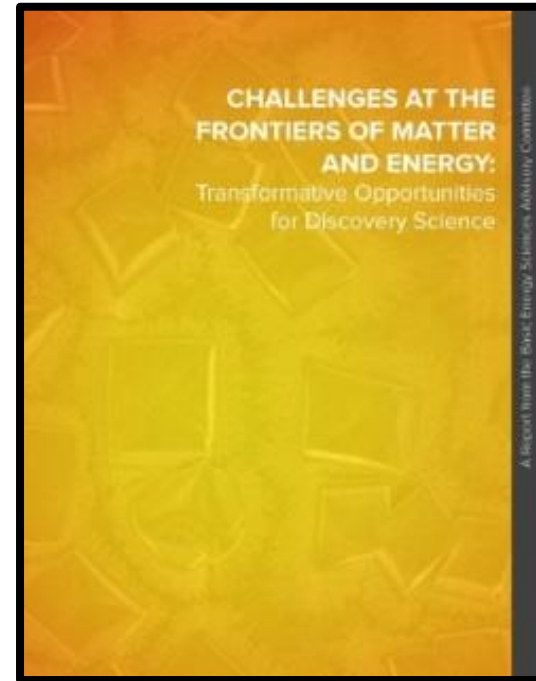
Key Documents Informing BES FY 2017 Budget Request



<http://energy.gov/quadrennial-technology-review-2015>

DOE Crosscuts:

- Advanced Materials
- Exascale Computing Initiative
- Subsurface Science, Technology, and Engineering



http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_report_print.pdf

Transformative Opportunities:

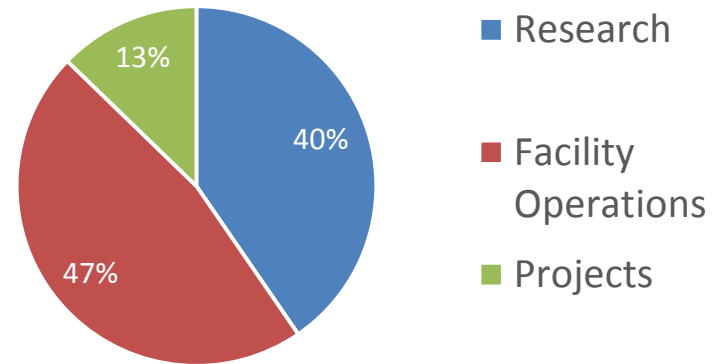
- Hierarchical architectures
- Non-equilibrium matter, non-ideal systems
- Coherence in light and matter
- Modeling and computation
- Imaging across multiple scales

Basic Energy Sciences

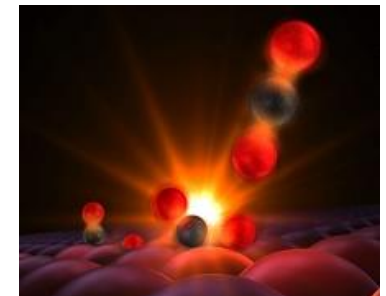
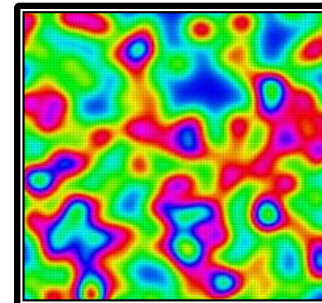
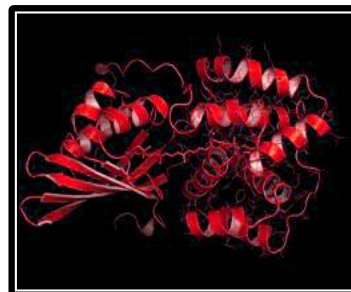
Understanding, predicting, and controlling matter and energy at the electronic, atomic, and molecular levels

- User facilities: X-ray light sources, neutron sources, and Nanoscience Research Centers.
- Research in materials science, chemistry, and geoscience
- 32 Energy Frontier Research Centers
- 2 Energy Innovations Hubs

FY 16 Omnibus






FY16 BES Total: \$1.849B




High Energy Physics

Understanding how the universe works at its most fundamental level

- Particle Physics Project Prioritization Panel (**P5**) report in May 2014 presents an actionable long-term strategy for U.S. particle physics that enables discovery and maintains the U.S. position as a global leader in particle physics.
- **Five intertwined science drivers**, compelling lines of inquiry that show great promise for discovery:

-  Use the **Higgs boson** as a new tool for discovery
-  Pursue the physics associated with **neutrino mass**
- Identify the new physics of **dark matter**
-  Understand **cosmic acceleration**: dark energy and inflation
- **Explore the unknown**: new particles, interactions, and physical principles

	Energy Frontier	Intensity Frontier	Cosmic Frontier
Higgs Boson	●		
Neutrino Mass		●	●
Dark Matter	●	●	●
Cosmic Acceleration			●
Explore the Unknown	●	●	●

- Science drivers identify the scientific motivation while the **Energy, Intensity, and Cosmic Research Frontiers** provide a useful categorization of experimental techniques

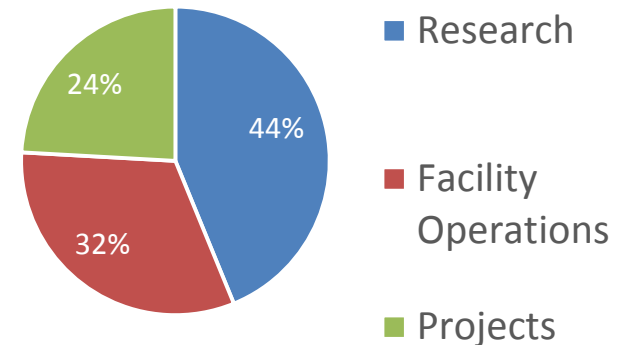


High Energy Physics

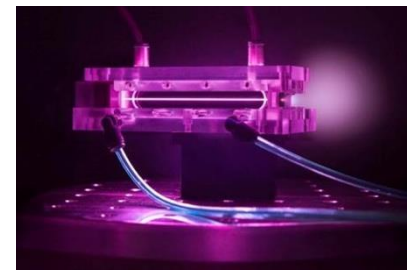
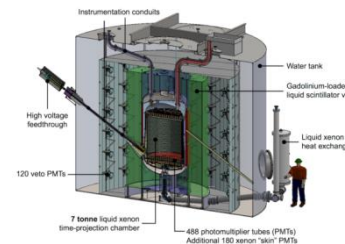
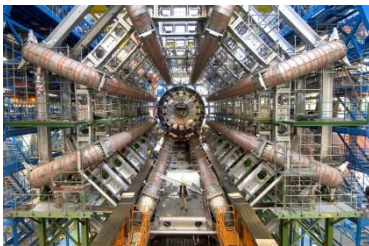
Understanding how the universe works at its most fundamental level, including exploring the elementary constituents of matter and energy, the interactions between them, and the nature of space and time.

- Research: Science Drivers from P5 Report: Higgs boson, neutrino mass, dark matter, cosmic acceleration, and exploring the unknown.
- User facilities and large-scale collaborative experiments at the energy, intensity, and cosmic frontiers, including the LHC, LBNF/DUNE, and LSST.
- Next-generation of accelerator technology and new application of accelerators for science and industry.

FY 16 Omnibus



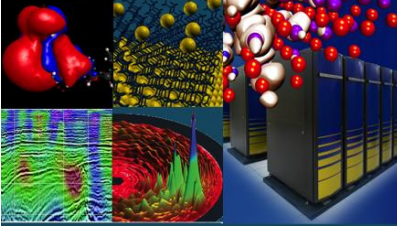
FY16 HEP Total: \$795M



Computational Capacity is Based on Requirements

“Lead with the Science”

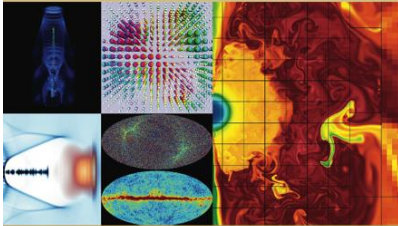
LARGE SCALE COMPUTING AND STORAGE REQUIREMENTS



Basic Energy Sciences

Report of the NERSC / BES / ASCR
Requirements Workshop
February 9 and 10, 2010

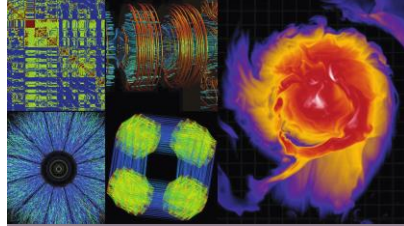
LARGE SCALE COMPUTING AND STORAGE REQUIREMENTS



High Energy Physics

Report of the NERSC / HEP / ASCR
Requirements Workshop
November 12 and 13, 2009

LARGE SCALE COMPUTING AND STORAGE REQUIREMENTS



Nuclear Physics

Report of the NERSC / NP / ASCR
Requirements Workshop
May 26 and 27, 2011

LARGE SCALE COMPUTING AND STORAGE REQUIREMENTS



Advanced Scientific Computing Research

Report of the NERSC / ASCR
Requirements Workshop
January 5 and 6, 2011

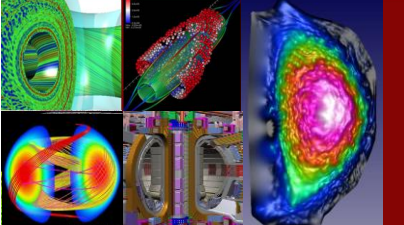
LARGE SCALE COMPUTING AND STORAGE REQUIREMENTS



Biological and
Environmental Research

Report of the NERSC/BES/ASCR
Requirements Workshop
May 7 and 8, 2009

LARGE SCALE COMPUTING AND STORAGE REQUIREMENTS



Fusion Energy Sciences

Report of the NERSC / FES / ASCR
Requirements Workshop
August 3 and 4, 2010

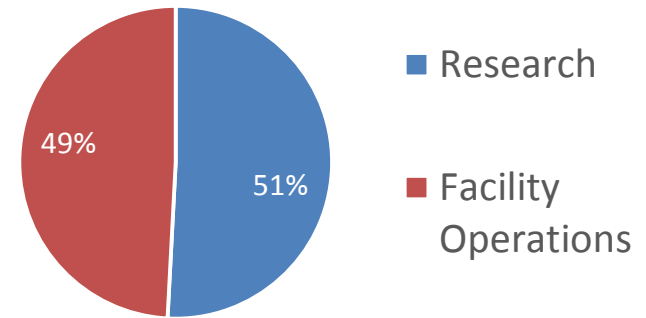


Advanced Scientific Computing Research

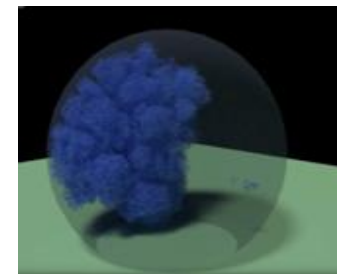
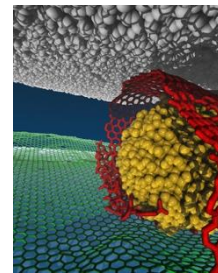
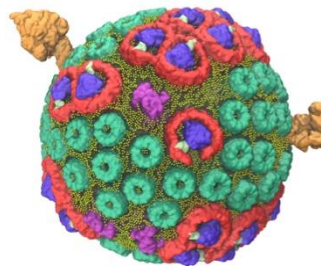
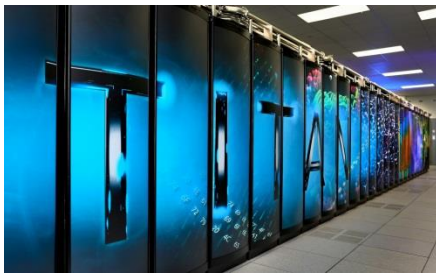
Discovering, developing, and deploying computational and networking capabilities for analysis, modeling, simulation, and prediction of complex phenomena

- High performance computing systems at: Oak Ridge and Argonne Leadership Computing Facilities, and the National Energy Research Scientific Computing Center.
- Research: applied math, computer science, high-performance networks (ESNet), and computational partnership (SciDAC) in support of next-generation HPC systems and applications, including exascale computing.

FY 16 Omnibus



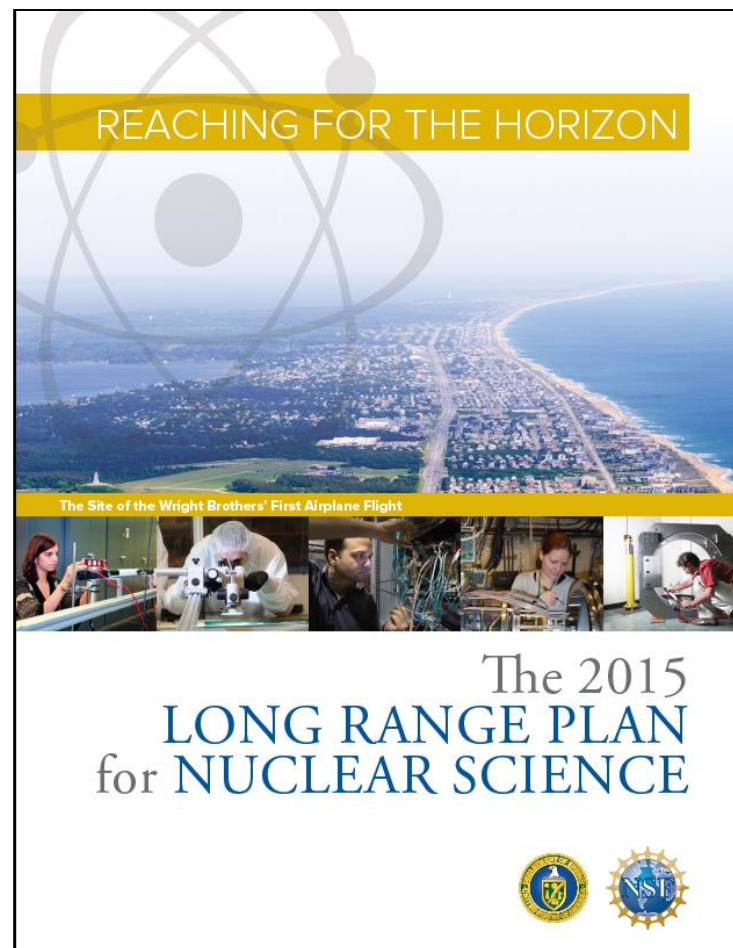
FY16 ASCR Total: \$621M



The 2015 Long Range Plan for Nuclear Science

Recommendations:

1. Capitalize on investments made to maintain U.S. leadership in nuclear science.
2. Develop and deploy a U.S.-led ton-scale neutrino-less double beta decay experiment.
3. Construct a high-energy high-luminosity polarized electron-ion collider (EIC) as the highest priority for new construction following the completion of FRIB.
4. Increase investment in small-scale and mid-scale projects and initiatives that enable forefront research at universities and laboratories.



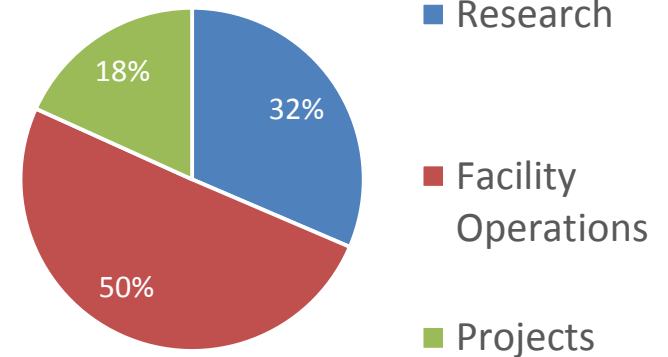
http://science.energy.gov/~media/np/nsac/pdf/2015LRP/2015_LRPNS_091815.pdf

Nuclear Physics

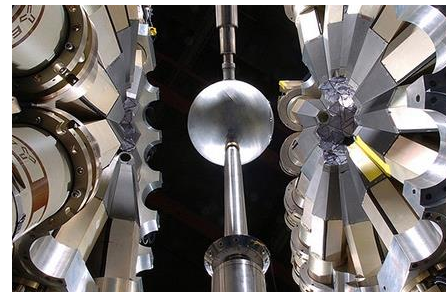
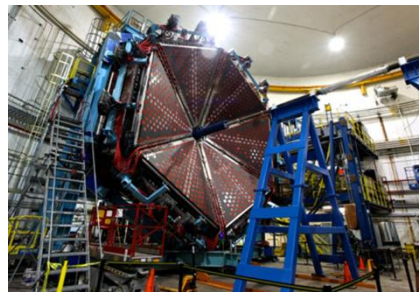
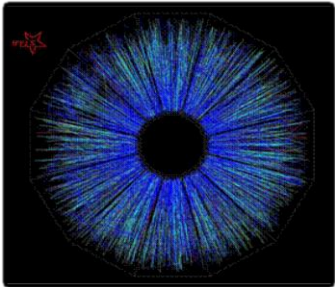
Discovering, exploring, and understanding all forms of matter.

- User facilities in heavy ion, medium energy, and low energy physics: ATLAS, RHIC, CEBAF, and FRIB.
- FRIB will dramatically expand the number of isotopes with known properties and enable research in nuclear structure, nuclear astrophysics, and fundamental symmetries.
- R&D for production of stable and radioactive isotopes crucial to science, technology, medicine, and homeland security.

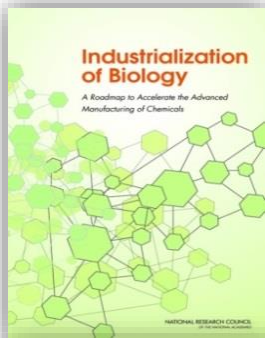
FY 16 Omnibus



FY16 NP Total: \$617M

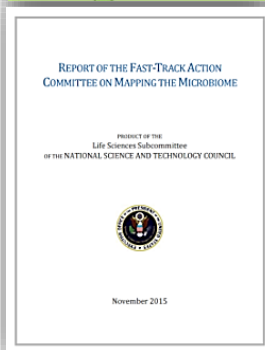


Key Documents Informing the BER FY 2017 Budget Request



<http://www.nap.edu/catalog/19001/industrialization-of-biology-a-roadmap-to-accelerate-the-advanced-manufacturing>

Biosystems Design efforts in plants and microbes underpinning development of clean energy



https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/ftac-mm_report_final_112015_0.pdf

The microbiome impacts on plant growth and development, availability of soil nutrients, and carbon cycle processes under changing climate conditions



<http://www.globalchange.gov/browse/reports/our-changing-planet-FY-2016>

Developing physical, chemical, and biological model components to simulate climate variability and change at regional and global scales.
Supports DOE crosscuts in Exascale Computing and the Energy-Water Nexus



U.S. DEPARTMENT OF
ENERGY

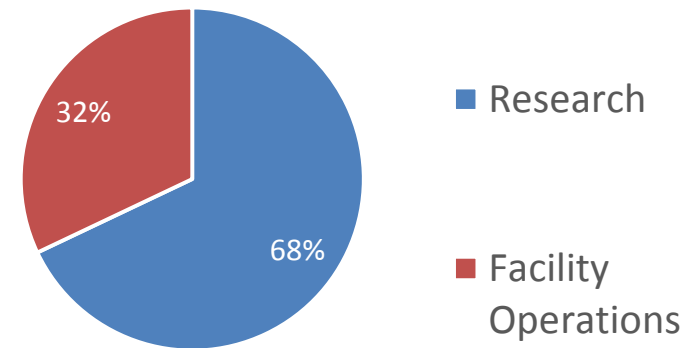
Office of
Science

Biological and Environmental Research

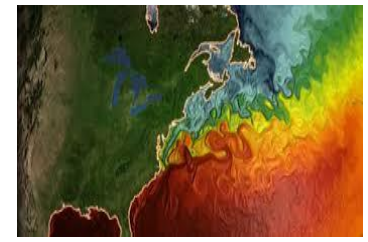
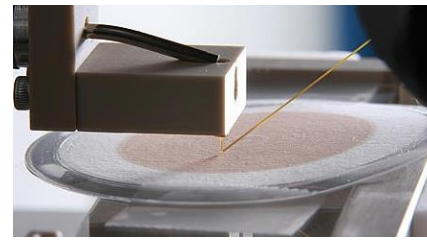
Understanding Complex Natural Systems Across Many Spatial and Temporal Scales by Coupling Theory, Observations, Experiments, Models, and Simulations

- Research: genomic science for sustainable bioenergy, carbon cycling, and bioremediation, and climate and environmental science to support development of predictive models.
- User facilities: Joint Genome Institute, Environmental Molecular Sciences Laboratory, Atmospheric Radiation Measurement Climate Research Facility
- Three multidisciplinary, multi-institutional Bioenergy Research Centers.

FY 16 Omnibus



FY16 BER Total: \$609M



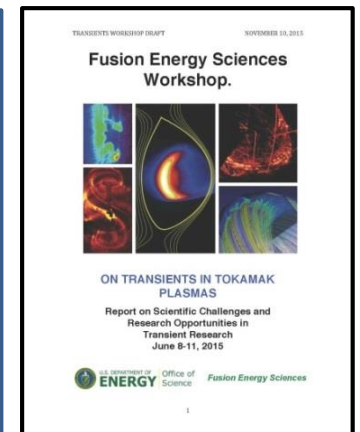
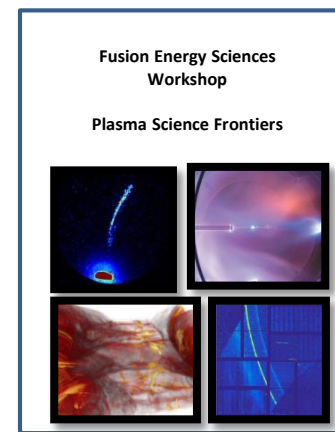
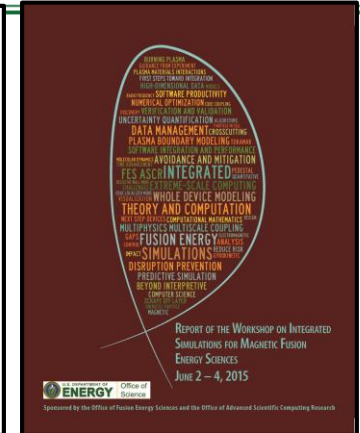
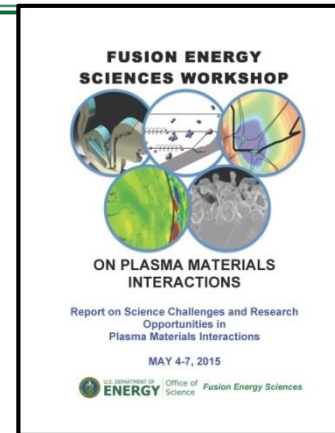
U.S. DEPARTMENT OF
ENERGY

Office of
Science

FES Community Engagement Workshops

- Following the FESAC *Strategic Planning and Priorities Report* (2014), FES undertook a series of four technical workshops in 2015:
 - Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences
 - Workshop on Transients
 - Workshop on Plasma Science Frontiers
 - Workshop on Plasma-Materials Interaction
- Each workshop is delivering a report that addresses scientific challenges and potential implementation options.

<https://www.burningplasma.org/activities/?article=FES%20Community%20Planning%20Workshops%202015>

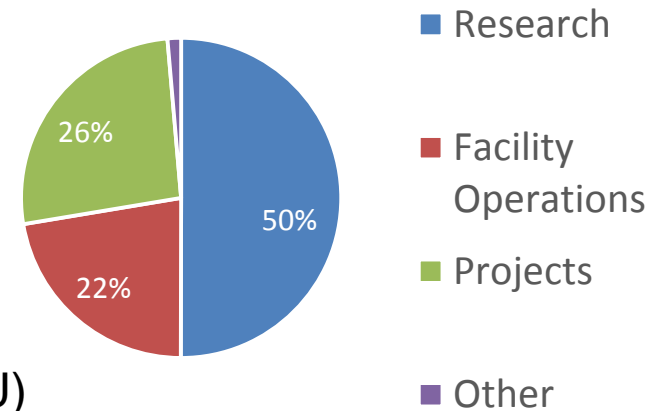


Fusion Energy Sciences

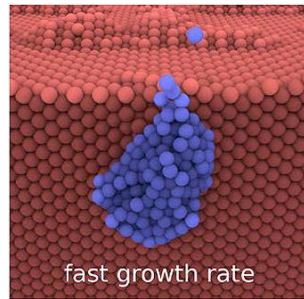
Expanding the fundamental understanding of matter at very high temperatures and densities and building the scientific foundation needed to develop a fusion energy source.

- User facilities: the NSTX-U (PPPL) and DIII-D Tokamak (General Atomics).
- Significant contributions to international fusion experiments, including EAST (China), KSTAR (Korea), W7-X stellarator (Germany).
- Contributions to the science and technology of ITER (EU)
- General plasma science and materials in extreme conditions.

FY 16 Omnibus



FY16 FES Total: \$438M



Office of Science Laboratories

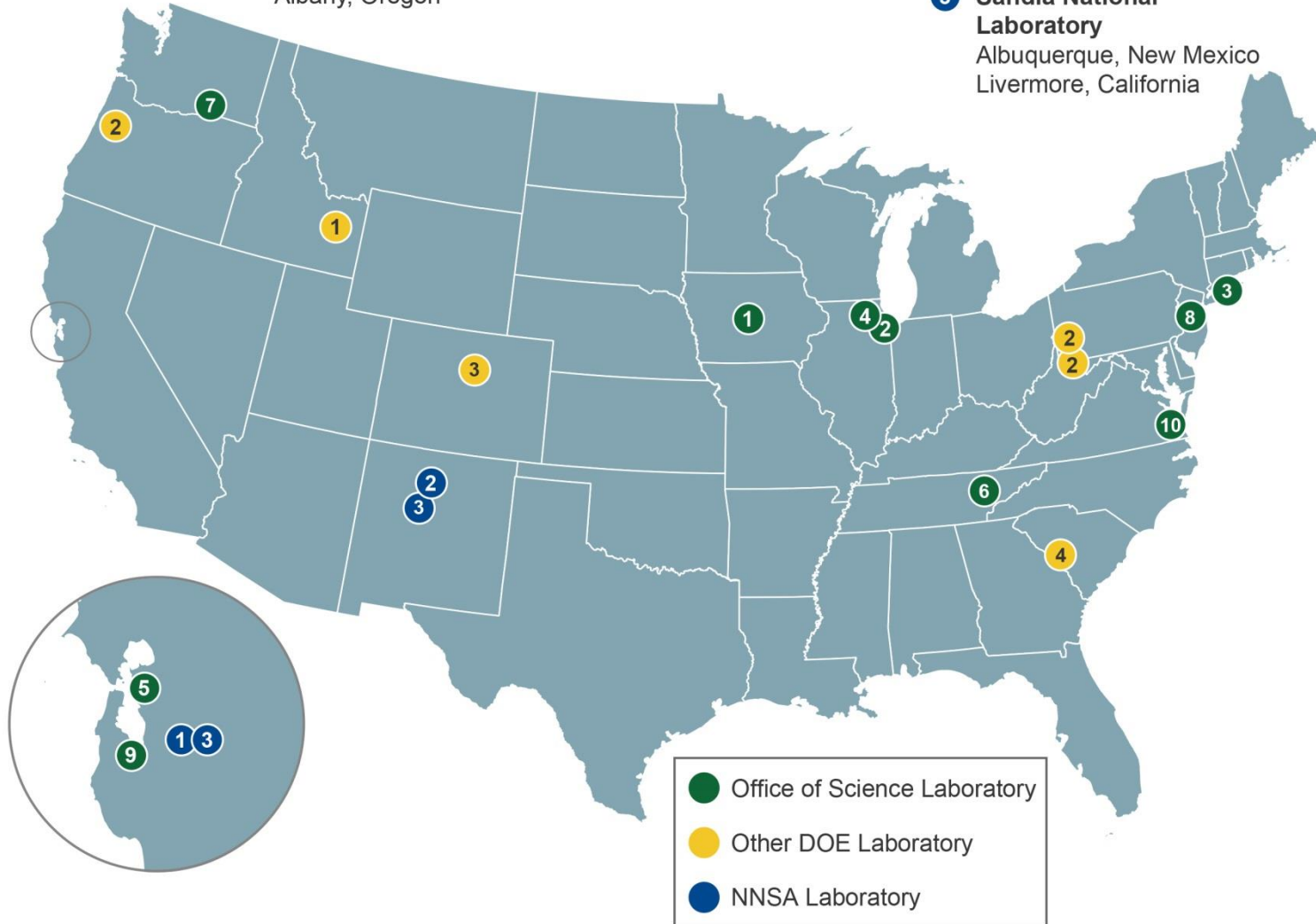
- 1 Ames Laboratory**
Ames, Iowa
- 2 Argonne National Laboratory**
Argonne, Illinois
- 3 Brookhaven National Laboratory**
Upton, New York
- 4 Fermi National Accelerator Laboratory**
Batavia, Illinois
- 5 Lawrence Berkeley National Laboratory**
Berkeley, California
- 6 Oak Ridge National Laboratory**
Oak Ridge, Tennessee
- 7 Pacific Northwest National Laboratory**
Richland, Washington
- 8 Princeton Plasma Physics Laboratory**
Princeton, New Jersey
- 9 SLAC National Accelerator Laboratory**
Menlo Park, California
- 10 Thomas Jefferson National Accelerator Facility**
Newport News, Virginia

Other DOE Laboratories

- 1 Idaho National Laboratory**
Idaho Falls, Idaho
- 2 National Energy Technology Laboratory**
Morgantown, West Virginia
Pittsburgh, Pennsylvania
Albany, Oregon
- 3 National Renewable Energy Laboratory**
Golden, Colorado
- 4 Savannah River National Laboratory**
Aiken, South Carolina

NNSA Laboratories

- 1 Lawrence Livermore National Laboratory**
Livermore, California
- 2 Los Alamos National Laboratory**
Los Alamos, New Mexico
- 3 Sandia National Laboratory**
Albuquerque, New Mexico
Livermore, California



Office of Science Laboratories Total FY15 \$5.5B, SC funding \$3.4B



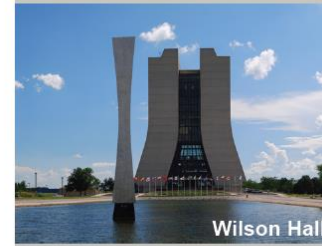
Berkeley, California
 202 acres and 90 buildings
 3,232 FTEs
 950 students & postdocs
 9,484 facility users
www.lbl.gov



Richland, Washington
 346 acres and 20 buildings
 4,308 FTEs
 628 students & postdocs
 2,022 facility users
www.pnnl.gov



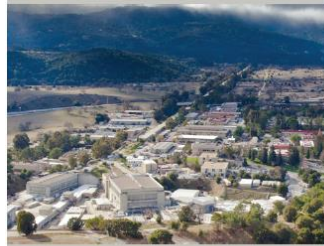
Ames, Iowa
 8 acres and 12 buildings
 310 FTEs
 162 students & postdocs
www.ameslab.gov



Batavia, Illinois
 6,800 acres and 366 buildings
 1,760 FTEs
 46 students & postdocs
 2,340 facility users
www.fnal.gov



Argonne, Illinois
 1,517 acres and 100 buildings
 3,412 FTEs
 620 students & postdocs
 7,396 facility users
www.anl.gov



Menlo Park, California
 426 acres and 147 buildings
 1,422 FTEs
 230 students & postdocs
 2,913 facility users
www.slac.stanford.edu



Oak Ridge, Tennessee
 4,421 acres and 195 buildings
 4,525 FTEs
 1,429 students & postdocs
 2,987 facility users
www.ornl.gov



Newport News, Virginia
 169 acres and 72 buildings
 673 FTEs
 62 students & postdocs
 1,380 facility users
www.jlab.org



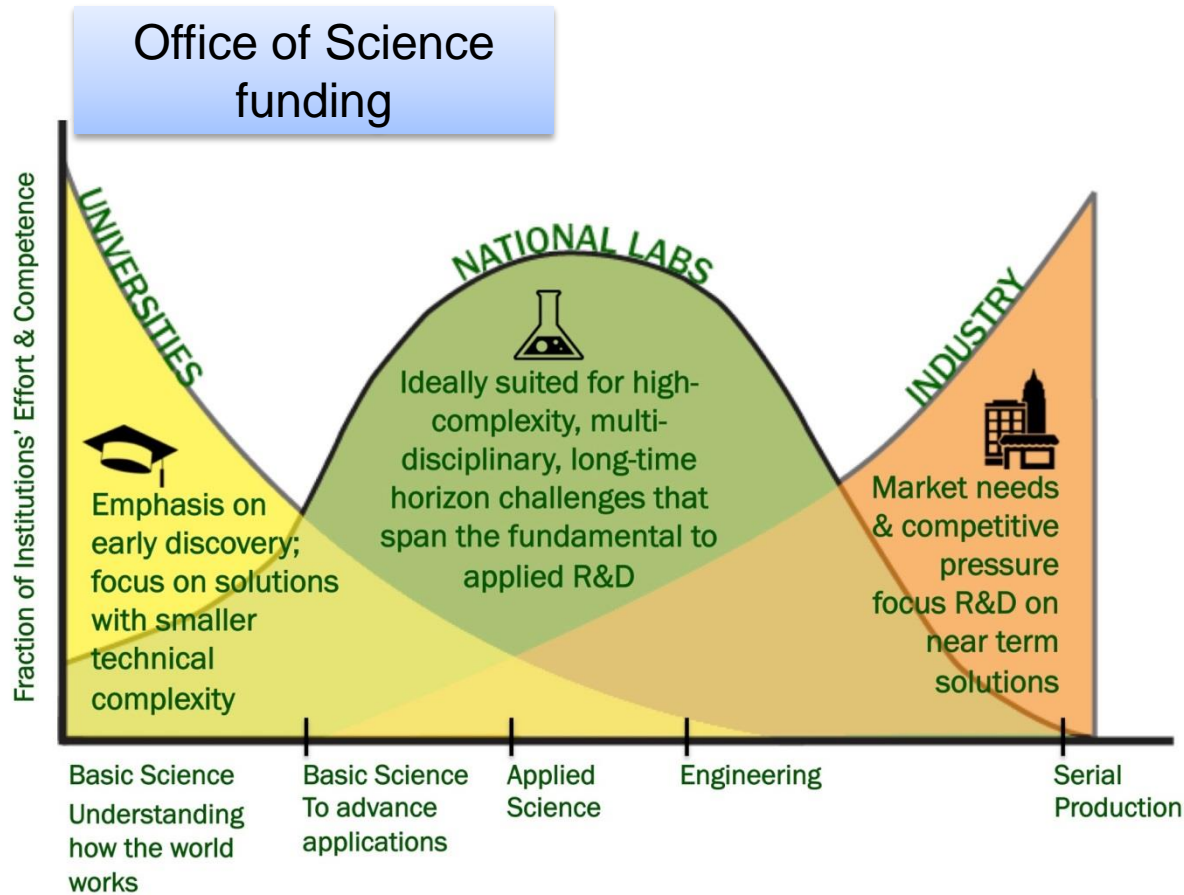
Princeton, New Jersey
 91 acres and 32 buildings
 431 FTEs
 59 students & postdocs
 290 facility users
www.pppl.gov



Upton, New York
 5,322 acres and 319 buildings
 2,788 FTEs
 557 students & postdocs
 4,090 facility users
www.bnl.gov

National Labs Address Multidisciplinary S&T Challenges

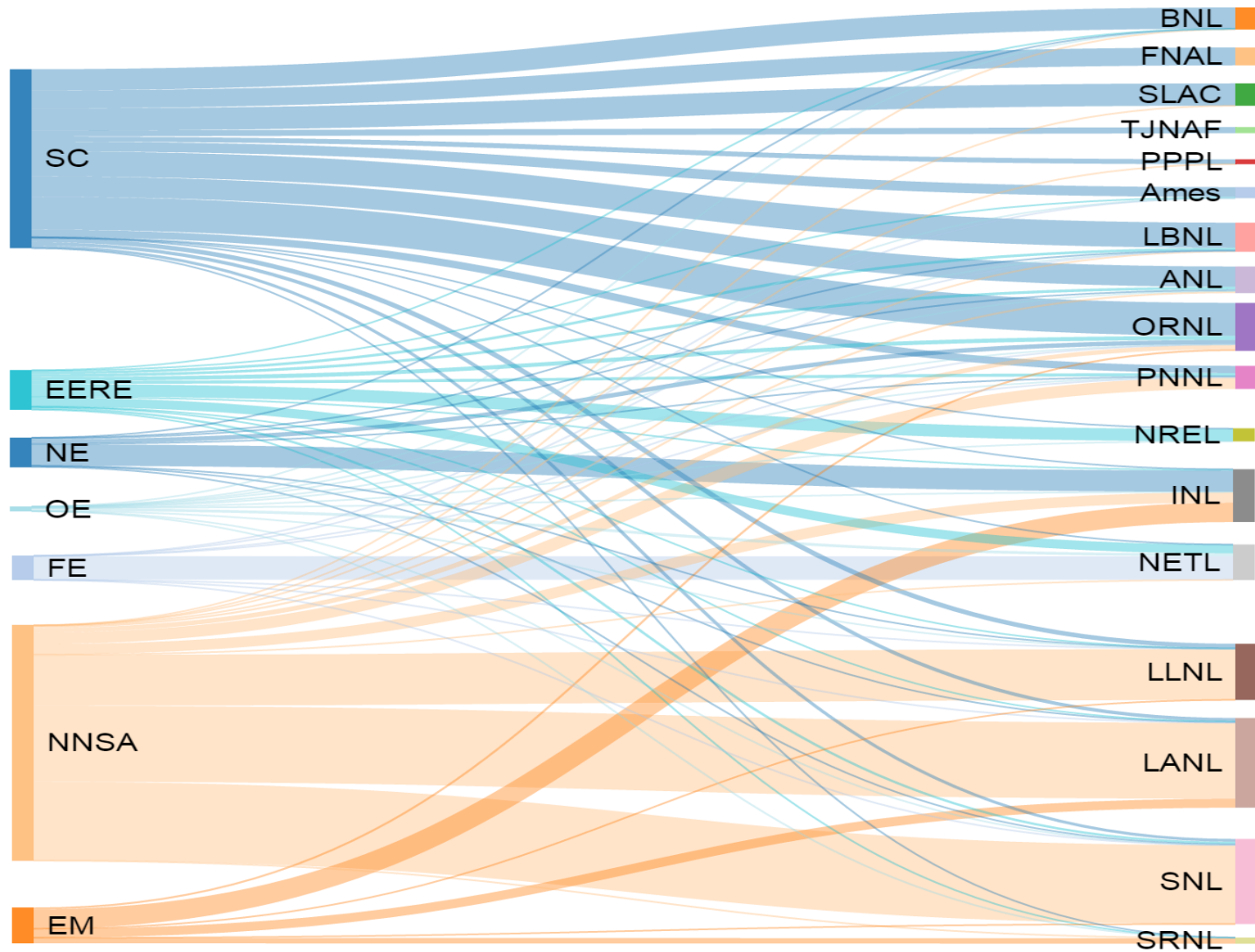
Most of the national labs have broader scope than Office of Science



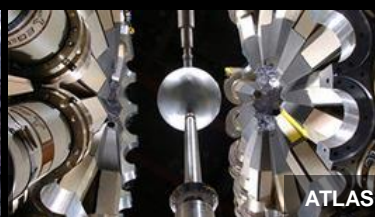
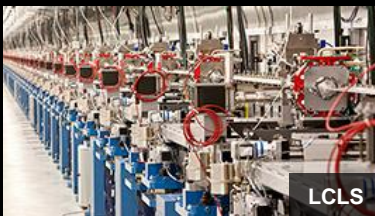
National Laboratory Directors Council



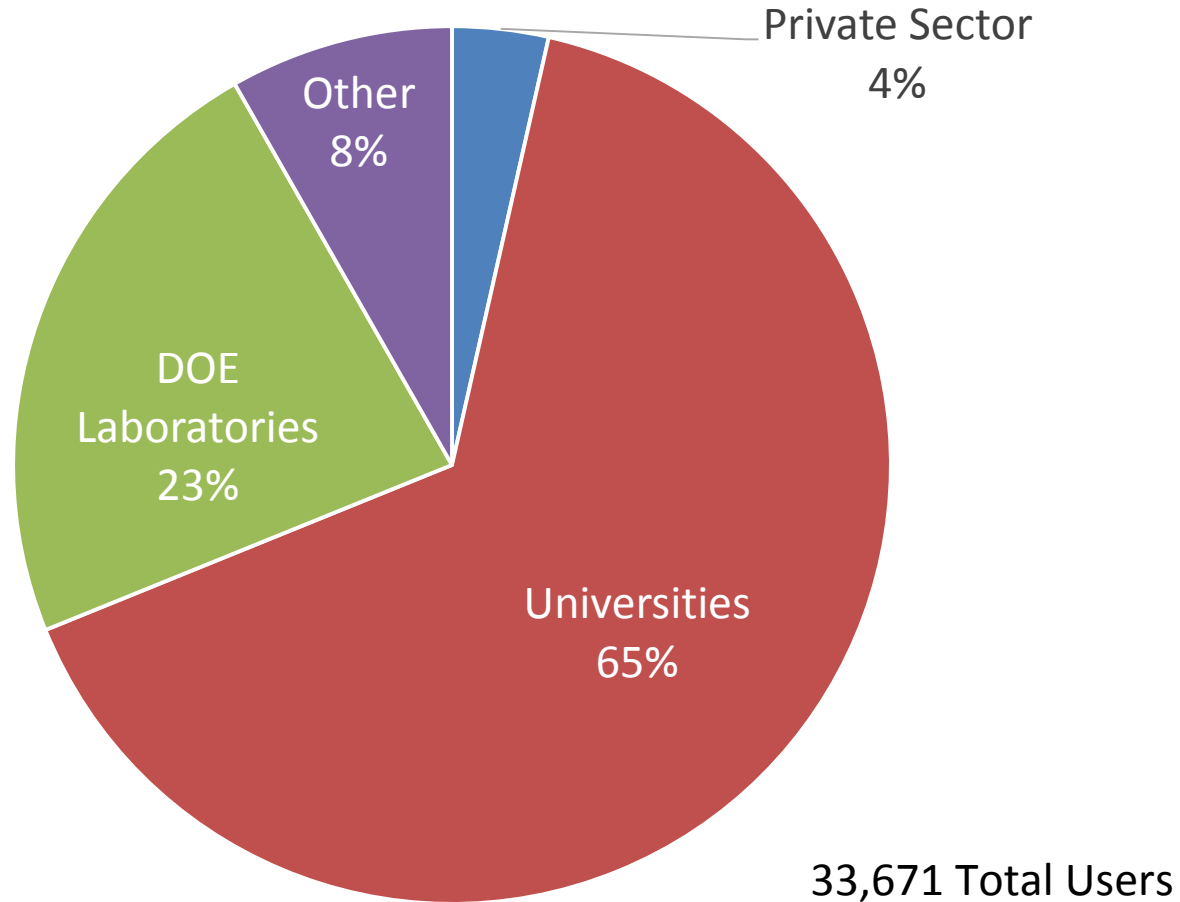
Flow of Funds between DOE Programs to Labs, 2015



FY 2016 28 user facilities



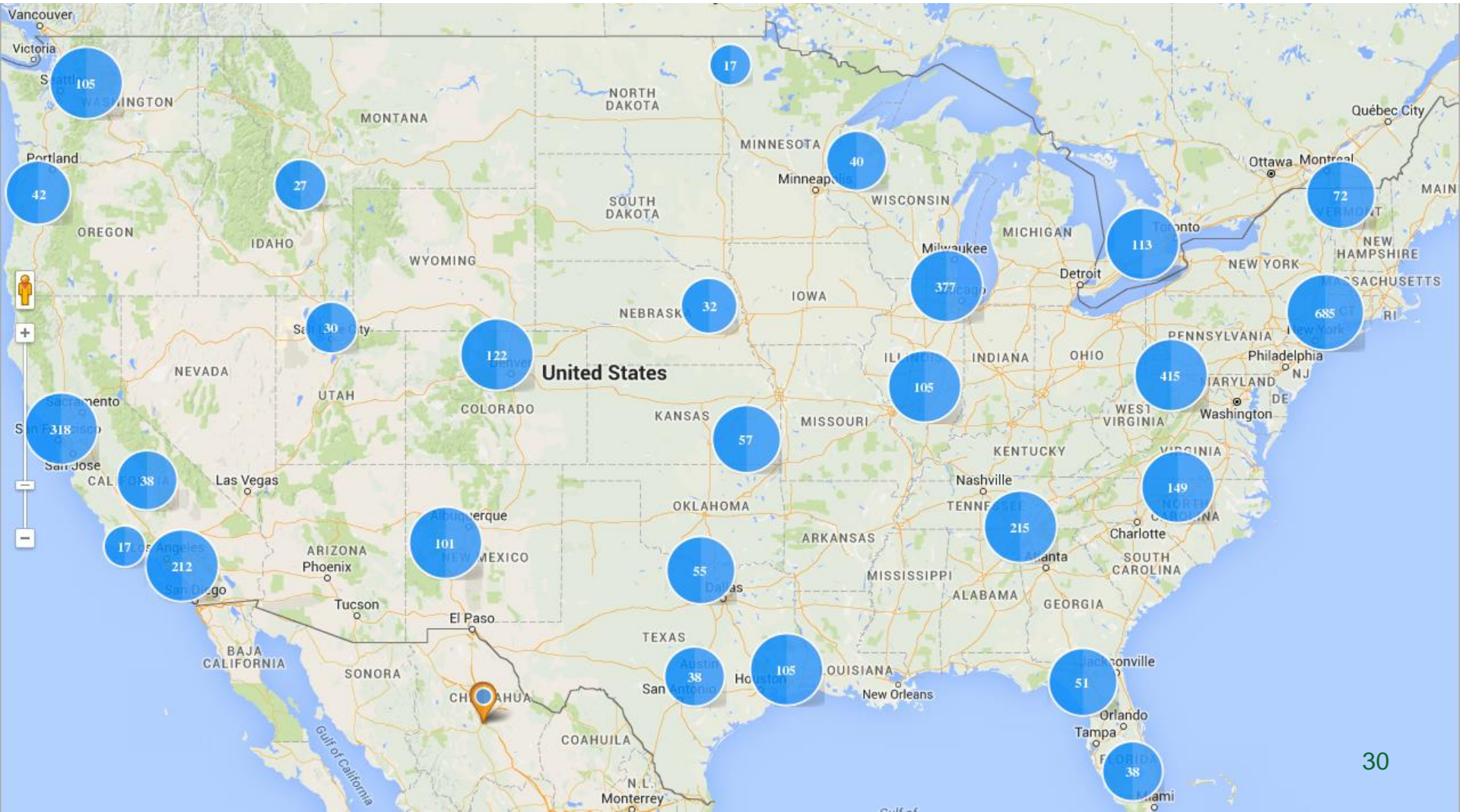
Office of Science User Facility Statistics FY14



Scientific User Facilities – Data on Users Across Country

<http://science.energy.gov/universities/interactive-grants-map/>

<http://science.energy.gov/user-facilities/user-statistics/>

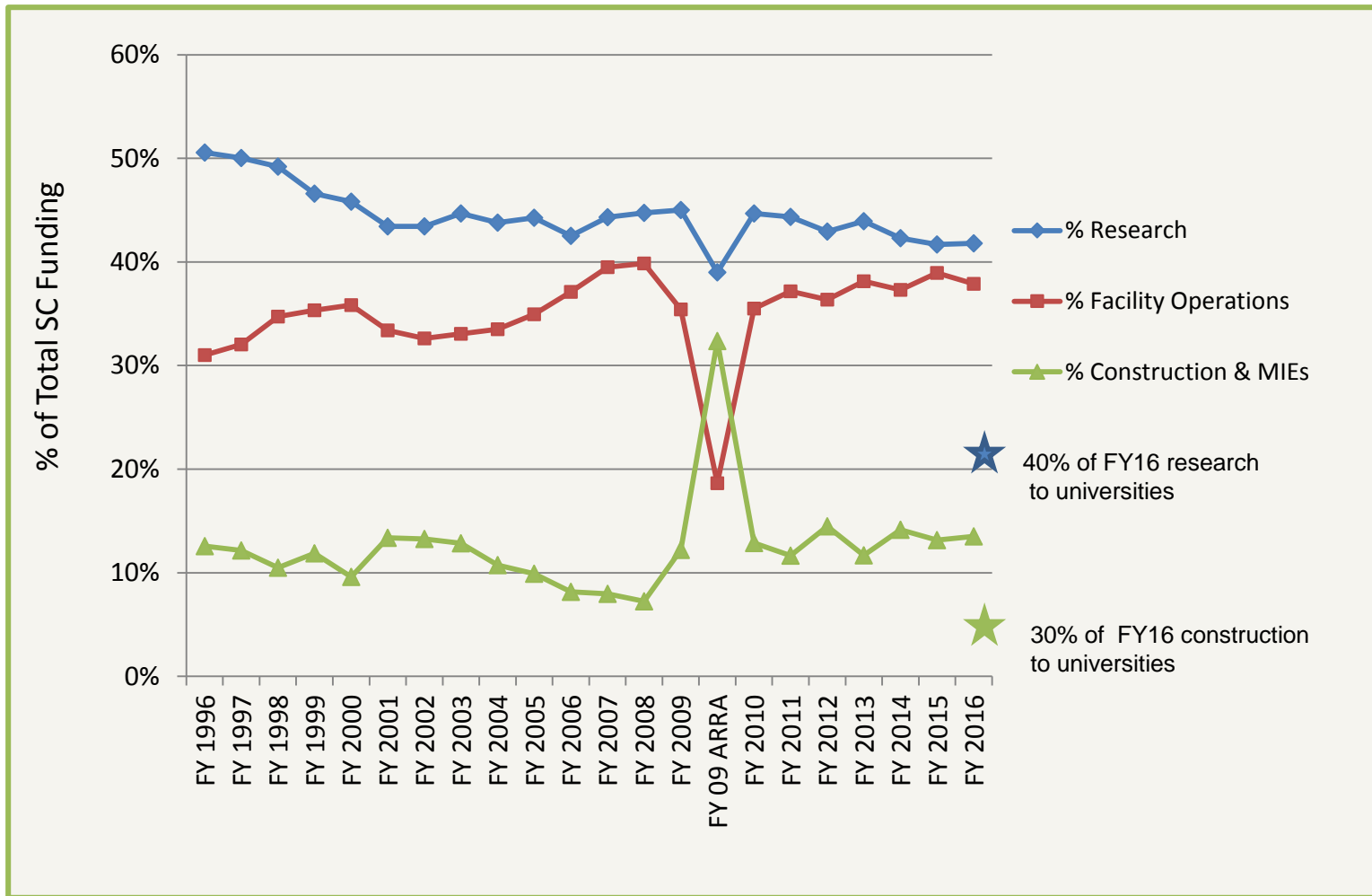


FY2017 Issues and Priorities

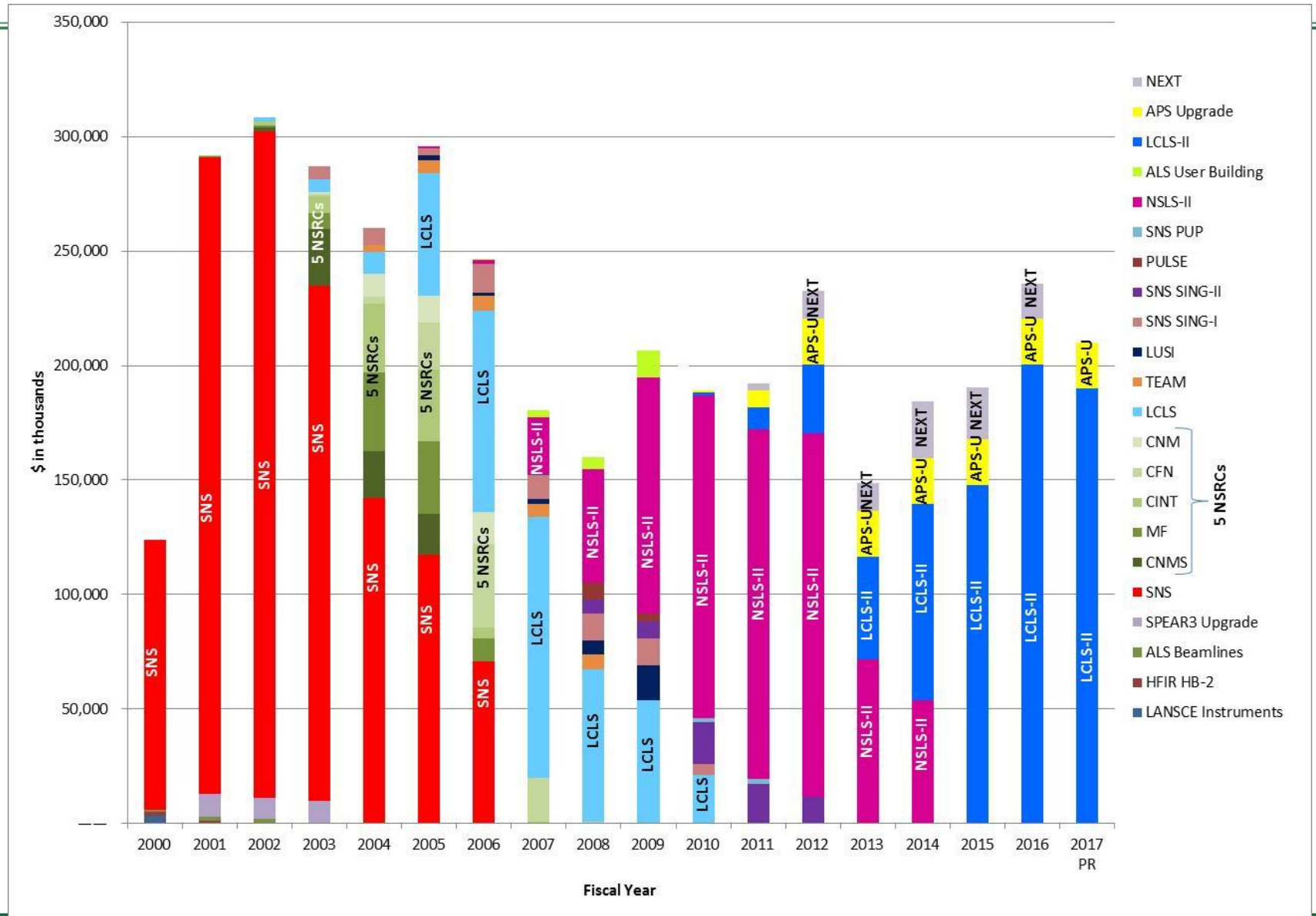
- **BALANCE - Research funding vs scientific user facilities construction vs operation**
- BALANCE - Discovery research vs science for clean energy and departmental crosscuts
- Exascale computing Project! National Strategic Computing Initiative
- International partnerships in Big Science
 - Defining moment in fusion sciences
 - LHC CMS, ATLAS upgrades at the same time as LBNF/DUNE
 - BESAC study of 5 proposed user facility upgrades



SC Investments in Research, Facilities, and Construction



BES Construction/MIE Funding Profile 2000 – 2017

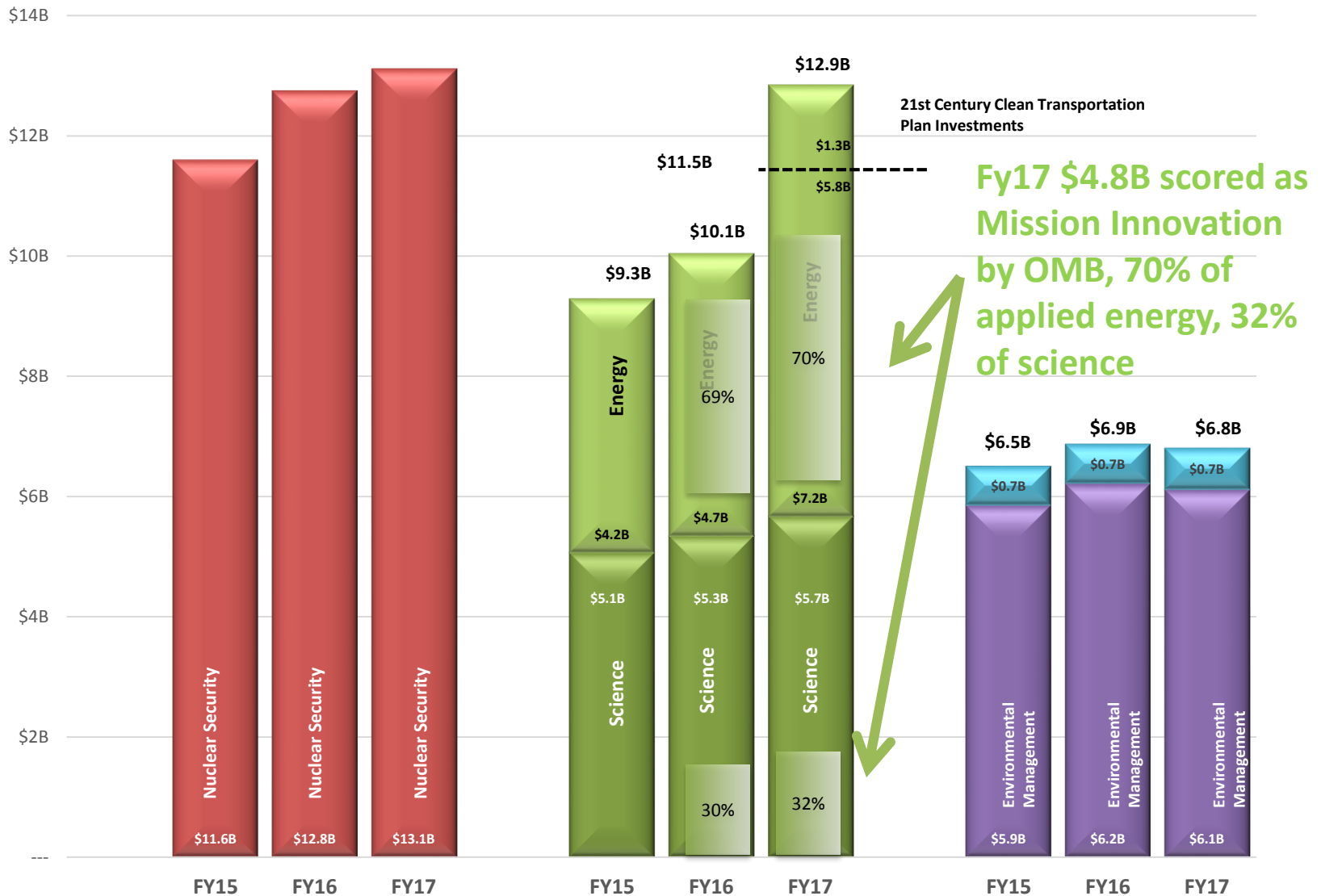


Fy2017 Issues and Priorities

- **BALANCE** - Research funding vs scientific user facilities construction vs operation
- **BALANCE** - Discovery research vs science for clean energy and departmental crosscuts
- Exascale computing Project! National Strategic Computing Initiative
- International partnerships in Big Science
 - Defining moment in fusion sciences
 - LHC CMS, ATLAS upgrades at the same time as LBNF/DUNE
 - BESAC study of 5 proposed user facility upgrades



DOE Mission Innovation R&D, FY 16 and 17



SC Investments for Mission Innovation

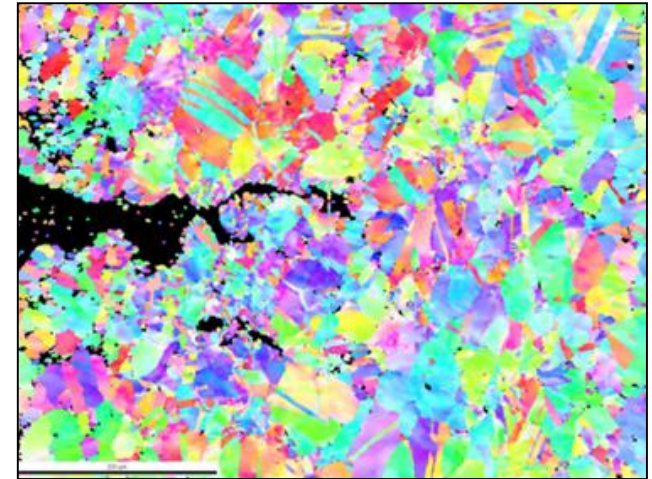
\$100M in new funding in FY 2017

ASCR (+\$10M)

- Computational Partnerships with EFRCs on solar, CO₂ reduction, catalysis, storage, subsurface, and biofuels; possibly new partnerships in wind and nuclear (\$10M)

BES (+\$51M)

- Energy Efficiency: Catalysts, modeled after nature's enzymes, that can operate at low-temperature and under ambient conditions; lightweight metallic materials; thermocaloric materials (\$34.4M)
- Materials for Clean Energy: Self-healing materials for corrosive and high radiation environments (next-gen corrosive-resistant materials based on experiments and multi-scale modeling; chemistry under harsh or extreme environments) (\$16.6M)



Analysis of cracks at the nanoscale

BER (+\$35M)

- Biosystems design (computationally design and then bio-engineer biosystems) to introduce beneficial traits into plants and microbes for clean energy applications (\$20M)
- Bioenergy Research Centers: New investments to translate 10 years of BRC research to industry (\$15M, \$5M per BRC)

FES (+4M)

- Whole-device fusion modeling and simulation using SciDAC partnerships (\$4M)



Fy2017 Issues and Priorities

- BALANCE - Research funding vs scientific user facilities construction vs operation
- BALANCE - Discovery research vs science for clean energy and departmental crosscuts
- **Exascale computing Project! National Strategic Computing Initiative**
- International partnerships in Big Science
 - Defining moment in fusion sciences
 - LHC CMS, ATLAS upgrades at the same time as LBNF/DUNE
 - BESAC study of 5 proposed user facility upgrades



The Opportunities and Challenges of Exascale Computing

Density Gradient
0.2 0.4 0.6 0.8
0.15

Vorticity Magnitude
0.00012 0.4 0.8 1.2 1.6 2

Summary Report of the
Advanced Scientific
Computing Advisory
Committee (ASCAC)
Subcommittee

Fall 2010

Top Ten Exascale Research Challenges

DOE ASCAC Subcommittee Report
February 10, 2014

Sponsored by the U.S. Department of Energy, Office of Science,
Office of Advanced Scientific Computing Research

Neuromorphic Computing: From Materials to Systems Architecture

Report of a Roundtable Convened to Consider Neuromorphic Computing Basic Research Needs

October 29-30, 2015
Gaithersburg, MD

Organizing Committee
Ivan K. Schuller (Chair),
University of California, San Diego
Rick Stevens (Chair),
Argonne National Laboratory and University of Chicago

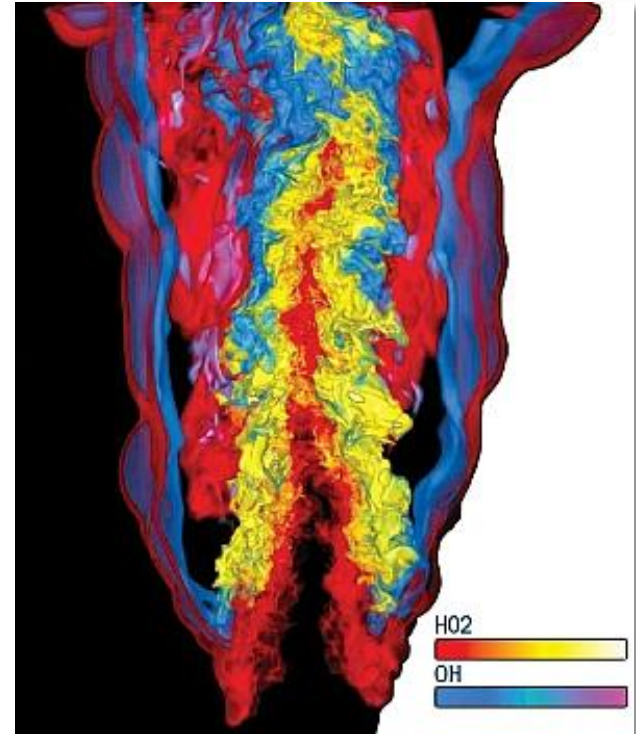
http://science.energy.gov/~media/ascr/ascac/pdf/reports/Exascale_subcommittee_report.pdf

<http://science.energy.gov/~media/ascr/ascac/pdf/meetings/20140210/Top10reportFEB14.pdf>

<http://science.energy.gov/bes/community-resources/reports/abstracts/#NCFMtSA>

DOE's Exascale Computing Initiative: Next Generation of Scientific Innovation

- **Departmental Crosscut – In partnership with NNSA**
- **“All-in” approach: hardware, software, applications, large data, underpinning applied math and computer science**
- **Supports DOE’s missions in national security and science:**
 - Stockpile stewardship – support annual assessment cycle
 - Discovery science – **next-generation materials; chemical sciences**
 - Mission-focused basic science in energy – next-generation **climate software**
 - Use current Leadership Computing approach for users
- **The next generation of advancements will require Extreme Scale Computing**
 - 100-1,000X capabilities of today’s computers with a similar physical size and power footprint
 - Significant challenges are power consumption, high parallelism, reliability
- **Extreme Scale Computing, cannot be achieved by a “business-as-usual,” evolutionary approach**
 - Initiate partnerships with U.S. computer vendors to perform the required engineering, research and development for system architectures for capable exascale computing
 - Exascale systems will be based on marketable technology – Not a “one off” system
 - Productive system – Usable by scientists and engineers



Extreme-Scale Science Data Explosion

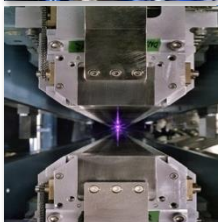


Genomics

Data Volume increases to 10 PB in FY21

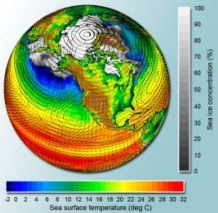


High Energy Physics
(Large Hadron Collider)
15 PB of data/year



Light Sources

Approximately
300 TB/day



Climate

Data expected to be
hundreds of 100 EB

Driven by exponential technology advances

Data sources

- Scientific Instruments
- Scientific Computing Facilities
- Simulation Results
- Observational data

Big Data and Big Compute

- Analyzing Big Data requires processing (e.g., search, transform, analyze, ...)
- Extreme scale computing will enable timely and more complex processing of increasingly large Big Data sets

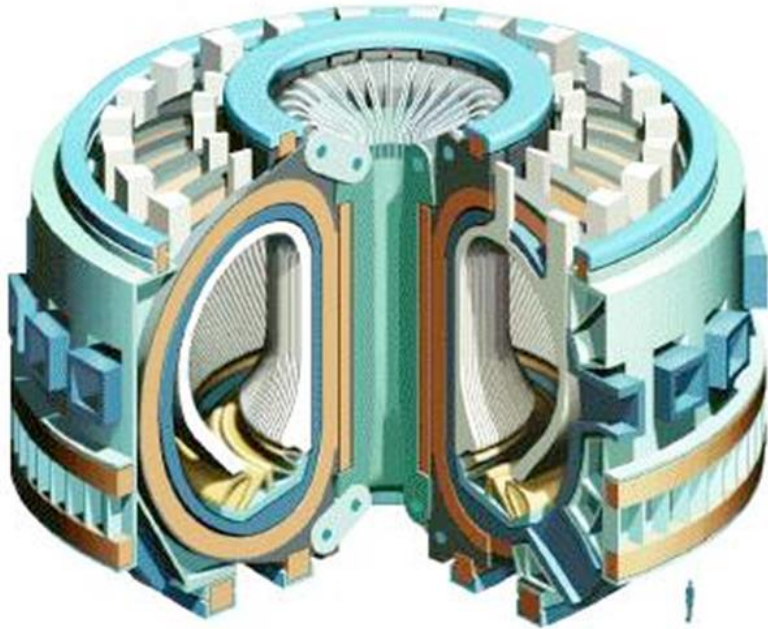


Fy2017 Issues and Priorities

- BALANCE - Research funding vs scientific user facilities construction vs operation
- BALANCE - Discovery research vs science for clean energy and departmental crosscuts
- Exascale computing Project! National Strategic Computing Initiative
- **International partnerships in Big Science**
 - Defining moment in fusion sciences
 - LHC CMS, ATLAS upgrades at the same time as LBNF/DUNE
 - BESAC study of 5 proposed user facility upgrades – international competitiveness



ITER Congressional Report

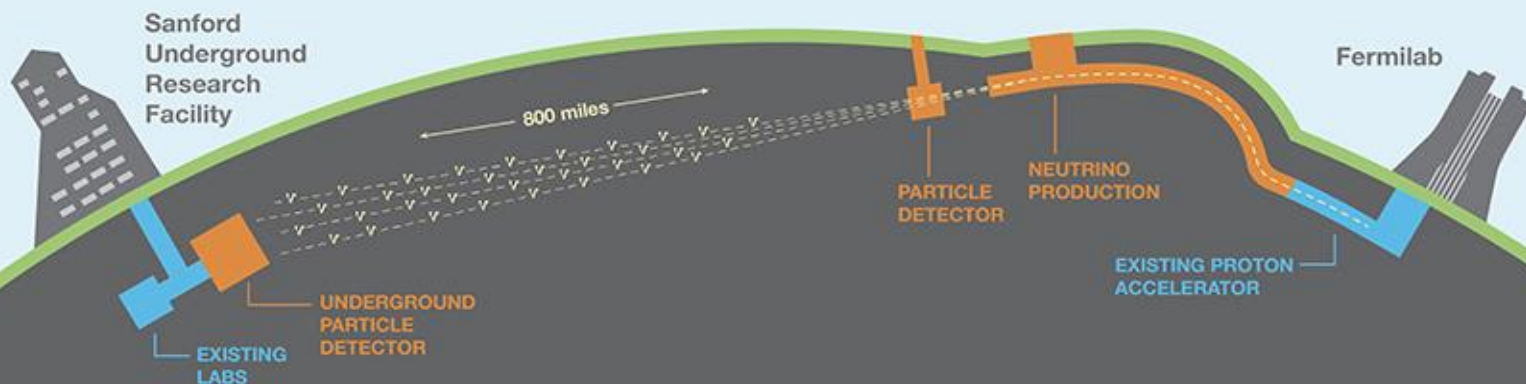


“...not later than May 2, 2016, the Secretary of Energy shall submit to the Committees on Appropriations of both Houses of Congress a report recommending either that the United States remain a partner in the ITER project after October 2017 or terminate participation, which shall include, as applicable, an estimate of either the full cost, by fiscal year, of all future Federal funding requirements for construction, operation, and maintenance of ITER or the cost of termination.”

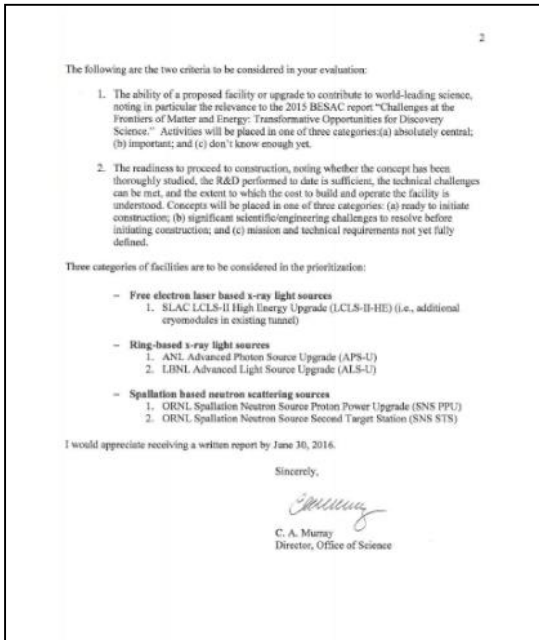
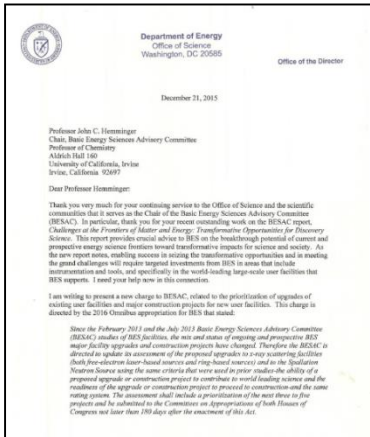


Long Baseline Neutrino Facility

- **P5 recommended LBNF as the centerpiece of a U.S.-hosted world-leading neutrino program**
 - P5 recognized LBNF as the highest-priority large project in its timeframe
- **The world's most intense neutrino beam will be produced at Fermilab and directed 800 miles through the earth to Lead, South Dakota**
 - Fermilab will lead this effort with a few international partners, most notably CERN
- **A very large (40 kiloton) liquid argon neutrino detector will be placed in the Homestake Mine in Lead, SD**
 - An international collaboration has been established for the Deep Underground Neutrino Experiment (DUNE)
 - The U.S. will contribute to the detector as part of the LBNF project



BESAC New Charge on Prioritization of Facility Upgrades



From: Dr. Cherry A. Murray (Director, Office of Science)

I am writing to present a new charge to BESAC, related to the prioritization of upgrades of existing user facilities and major construction projects for new user facilities.

The following are the two criteria to be considered in your evaluation:

1. The ability of a proposed facility or upgrade to contribute to world-leading science, noting in particular the relevance to the 2015 BESAC report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." Activities will be placed in one of three categories: (a) absolutely central; (b) important; and (c) don't know enough yet.
2. The readiness to proceed to construction, noting whether the concept has been thoroughly studied, the R&D performed to date is sufficient, the technical challenges can be met, and the extent to which the cost to build and operate the facility is understood. Concepts will be placed in one of three categories: (a) ready to initiate construction; (b) significant scientific/engineering challenges to resolve before initiating construction; and (c) mission and technical requirements not yet fully defined.

