Quadrennial Technology Review-2015

Chapter 10: Enabling Capabilities for Science and Energy

Public Webinar

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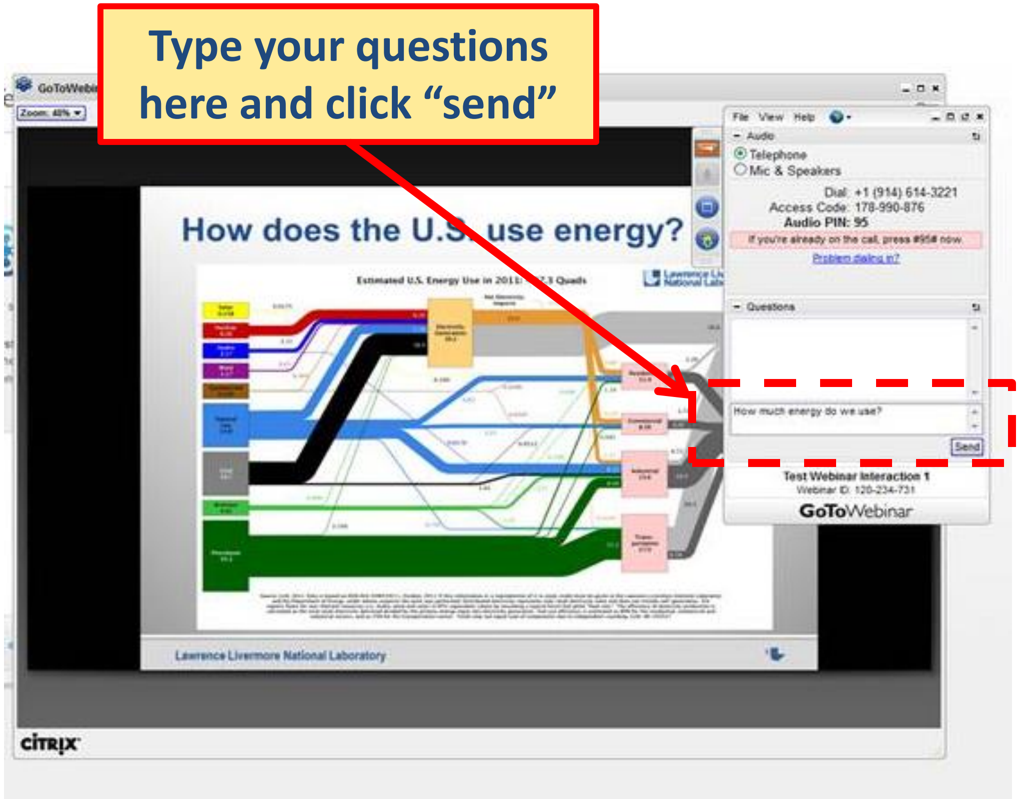
Webinar Logistics

- Due to the large number of expected participants, the audio and video portions of this webinar will be a “one way” broadcast. Only the organizers and QTR authors will be allowed to speak.

- Submit clarifying questions using the GoToWebinar control panel. Moderators will respond to as many questions as time allows. Substantial input regarding chapter content should be submitted by email to: DOE-QTR2015@hq.doe.gov



QTR 2015 Chapter Outline

Introduction

1. Energy Challenges
2. What has changed since QTR 2011
3. Energy Systems and Strategies

Assessments

4. Advancing Systems and Technologies to Produce Cleaner Fuels
5. Enabling Modernization of Electric Power Systems
6. Advancing Clean Electric Power Technologies
7. Increasing Efficiency of Buildings Systems and Technologies
8. Increasing Efficiency and Effectiveness of Industry and Manufacturing
9. Advancing Clean Transportation and Vehicle Systems and Technologies

10. Enabling Capabilities for Science and Energy

Integrated Analysis

11. U.S. Competitiveness
12. Integrated Analysis
13. Accelerating Science and Energy RDD&D
14. Action Agenda and Conclusions; Web-Appendices
    Web Appendices

Chapter Overview

- The Office of Science is the largest federal sponsor of basic research in the physical sciences and provides the scientific community with the most advanced tools of modern science, from high intensity light sources to atmospheric observation capabilities to high performance computers.
- Chapter 10 will provide readers with an overview of the capabilities stewarded by the Office of Science that support advances in basic research and applied research critical to the mission of the Office of Science and Department of Energy. This review can be divided into two equally important components:
  - The *Why* and *How* of the Office of Science – Why do we support this suite of facilities, what are the science drivers behind these capabilities, and how do we develop and maintain this portfolio?
  - The *What* of the Office of Science – What are the capabilities that we support, and what do they uniquely provide to the community?
- The capabilities included in this survey are *user facilities* - federally sponsored research facilities openly available for use to advance scientific or technical knowledge.

Chapter Outline

1. Introduction
2. The Office of Science
    1. Mission
    2. Historical Context
    3. Defining the Research Agenda
    4. User Facilities
3. Multi-disciplinary, Multi-scale Research
    1. Role of the DOE National Laboratories
    2. Novel Funding Modalities
    3. Coordination between Basic and Applied R&D

Chapter Outline

4. Understanding and Controlling Matter at the Atomic Scale
    1. Basic Energy Sciences
        1. X-ray Light Sources
        2. Neutron Scattering Facilities
        3. Nanoscale Science Research Centers
    2. Biological and Environmental Research
        1. Environmental Molecular Science Laboratory
        2. Joint Genome Institute
        3. Atmospheric Radiation Measurement Facility
5. Modeling and Simulation of Complex Systems
6. Fusion

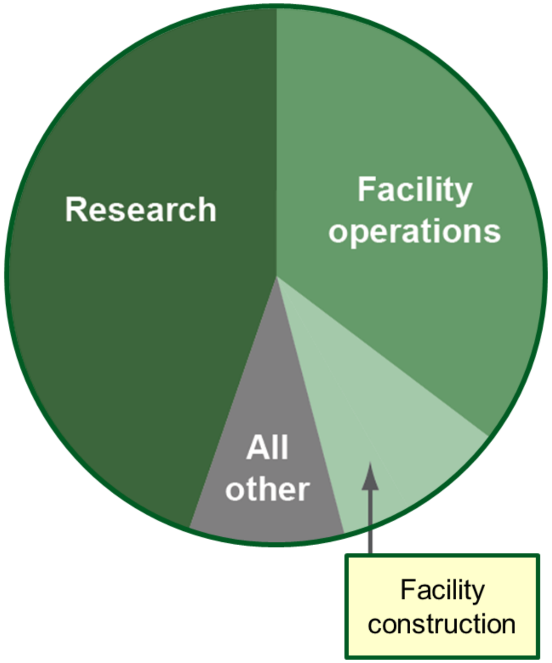
2. Office of Science
2.1 Mission

- The Office of Science's mission is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy economic, and national security of the United States.

- Support for *research* probing the fundamental questions within its core disciplines.
  - 22,000 Ph.D. scientists, grad students, engineers, and support staff at more than 300 institutions, including all17 DOE labs;
  - 47% of the U.S. Federal support of basic research in the physical sciences;
  - U.S. and world leadership in high-performance computing and computational sciences;
  - Major U.S. supporter of physics, chemistry, materials sciences, and biology for discovery science and for energy sciences;
  - More than 100 Nobel Prizes during the past 6 decades—more than 20 in the past 10 years.

- Support for *scientific user facilities*
  - The world's largest collection of scientific user facilities operated by a single organization in the world (>30), used by nearly 28,000 researchers from academia, industry, and labs each year.

FY 2015 Appropriations
$5.1 billion



2.2 Historical Context

Intent: Provide a history of and the context for the policies used by the Office of Science to develop its agenda for discovery science and facilities investment.

- The suite of capabilities currently supported by the Office of Science has it's origins in the Manhattan Project and the Atomic Energy Commission.
- The mission to support nuclear R&D required tools on a scale requiring the government to construct and operate them. The AEC created a series of national laboratories to provide the physical and human infrastructure to host and operate these machines.

Credit: Lawrence Berkeley National Laboratory

- The user facility model for the emerging laboratory-based computational and experimental capabilities started in the 60's and 70's as the scope of the mission was expanded to non-nuclear energy science and technology research.
- Consolidation of all federal energy-related research, policy and regulation in the Department of Energy led to formation of the Office of Energy Research (OER) with a Presidential-appointed Director as the steward for the basic science research portfolio.
- OER became the Office of Science in 1998, but the goals remained the same – basic science that is mission-relevant, collaborative, and focused on tackling *big challenges* with *big science* – using the large-scale tools that push the frontiers of science and innovation.

2.3 Developing the SC Portfolio

Intent: Describe how the Office of Science utilizes stakeholder input to identify opportunities and develop investment priorities.

- The continual development of the R&D portfolio leverages the deep scientific knowledge of its diverse stakeholder community.
  - Scientific and technical workshops (right);
  - Federal Advisory Committees of the SC program offices;
  - Interagency working groups (OSTP/NSTC; Congressionally mandated; informal/agency initiated);
  - Studies from the National Academies and other distinguished, independent science organizations;
  - DOE laboratory input (including the *Annual Lab Plans*);
  - Intra DOE working groups;
  - Solicited and unsolicited research proposals.

- Decisions are made with consideration of a broad range of input.
  - Consideration of Secretary and Administration priorities;
  - Consideration of Congressional priorities;
  - Consideration of interagency efforts/plans;
  - Identification of priorities for each program office and across SC;
  - State of current research and facilities (via external peer review);
  - Scientific and leadership opportunities;
  - Annual budget planning.

2.4 User Facilities in the Office of Science

Intent: Summarize the Office of Science definition of a user facility and describe the importance of open access and merit review of proposals to the user facility model.

- How is a user facility defined by the Office of Science and what requirements does the facility have once designated?
  - Open access for non-proprietary work;
  - Merit review of the proposed work;
  - Sufficient resources to support the users;
  - Unique capabilities that do not compete with the private sector.
- Non-SC User Facilities and Shared R&D Facilities.
- Accessing Facilities.
  - What are the general policies for an interested user?
  - General users and partner users.
  - Policies for the industrial user base.

3 Multi-disciplinary, Multi-scale Research
3.1 Role of the DOE Laboratories

- The 17 DOE national laboratories provide the nation with strategic scientific and technological capabilities by:
  - Executing long term S&T missions.
  - Developing unique, multi-disciplinary capabilities beyond the scope of academic and industrial institutions.
  - Developing and sustaining critical S&T capabilities.
- DOE laboratories house and operate the suite of user facilities (right), providing a staff of expert scientists and technicians to support the user community and develop the capabilities.
- The Office of Science collaborates with the labs to develop the long range vision for their institutions.

3.2 Novel Funding Modalities

Intent: Describe the Center and Hub funding models and their relationship to the core ideas in chapter 10 – leveraging unique capabilities for science and energy and tackling big challenges through collaborative research.

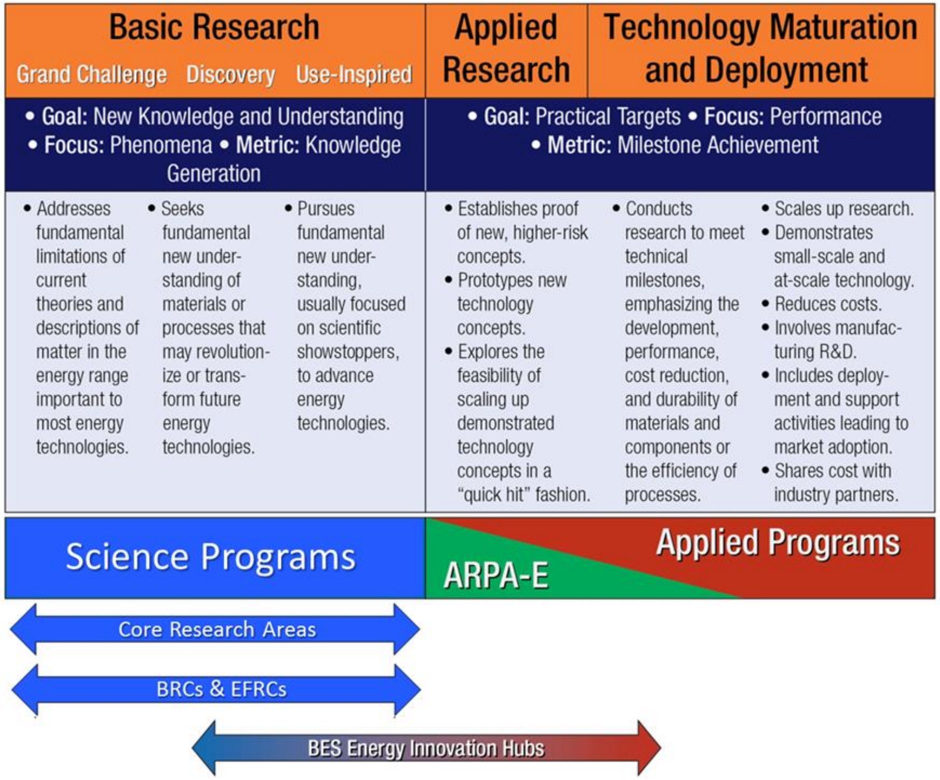
- DOE has initiated strategic funding modalities to promote collaborative, multi-disciplinary energy science. The three current programs are:
  - Energy Frontier Research Centers (36)
  - Energy Innovation Hubs (4)
  - Bioenergy Research Centers (3)
- While each modality has a unique structure and modes of operation, the overarching goal is to rapidly enable the innovative fundamental energy science research that will form the foundation for the transformative energy technology of the future.

	Investigators and Their Institutions	Period of Award and Management	Typical Annual Award Amount	Core Motivation and Research Focus
Energy Frontier Research Centers	Self-assembled groups of about 15 to 25 senior investigators. Led by universities, DOE laboratories, nonprofits, and industry, often with teaming across institutions.	Four years with possible 4-year renewal (pending appropriations). Managed by BES.	\$2M to \$4M	Fundamental research requiring multiple investigators from several disciplines, often with a clear link to new energy technologies. Research focused among a large set of basic research needs developed with community input.
Energy Innovation Hubs	Large group spanning basic and applied R&D. Led by universities, DOE laboratories, industry, or nonprofits, with extensive teaming across institutions.	Five years with possible 5-year renewal. Managed by a single DOE office but with broad coordination across DOE. BES manages the Fuels from Sunlight Battery Energy Innovation Hubs.	About \$22M in year one (with up to \$10M for infrastructure but no new construction). Up to \$25M/year in year two to five.	Purpose-driven research, integrating across basic and applied research toward commercialization. Generally, DOE determines the topical areas addressed by the hubs, and funding opportunity announcements (FOAs) are specific.
Bioenergy Research Centers	Three large, multi-disciplinary groups focused on the basic research challenges to cost effectively produce biofuels and bioproducts from plant biomass. Led by universities or DOE laboratories with extensive teaming across academia, national laboratories, and industry.	Five years with a possible 5-year renewal. All three bioenergy research centers were renewed for a second 5-year period in 2012. Managed by BER.	\$25M per year for each center.	Accelerate transformational breakthroughs in basic science needed for the development of cost effective, sustainable technologies to make production of cellulosic biofuels and bioproducts commercially viable on a national scale. Strong commitment to transferring basic science breakthroughs to the private sector through direct partnerships, collaborative affiliations, and the development and licensing of intellectual property.

3.3 Coordination between Basic and Applied R&D

Intent: Provide an overview, with examples, of the different mechanisms by which the Office of Science and the applied engineering programs coordinate activities.

- The Office of Science supports the effort to coordinate basic and applied technology R&D programs through a variety of activities, including:
  - Coordination working groups;
  - Joint PI meetings;
  - Focused tech teams;
  - Co-organized scientific and technical workshops;
  - Coordinated R&D programs – SBIR/STTR
- Specific examples from the Basic Energy Sciences , Biological and Environmental Research, and Advanced Scientific Computing Research programs will be noted.



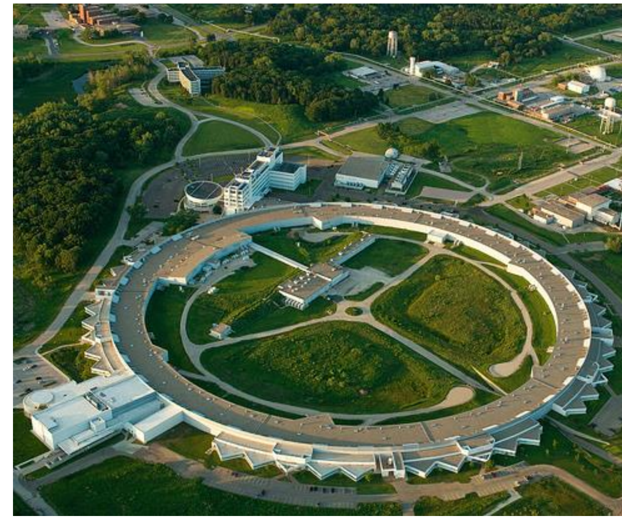
Source: 2014 Research Highlights, Basic Energy Science, Office of Science.

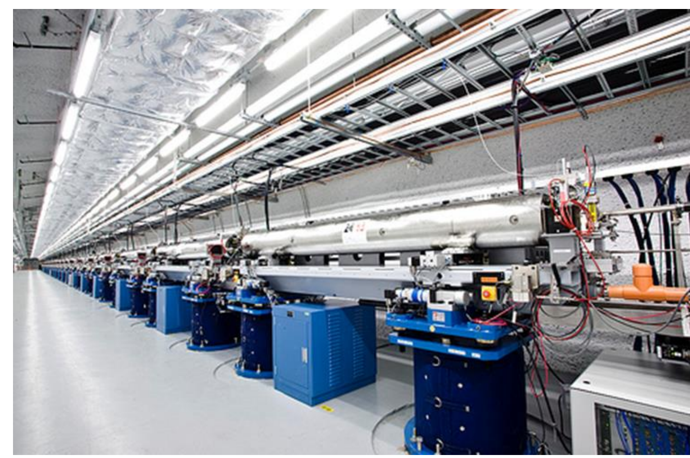
Format for Survey of Enabling Capabilities

- The survey of enabling capabilities will address the following four points for each facility or class of facilities. They are approximately ordered by importance:
  - What were the science drivers, goals, and/or grand challenges that led the Office of Science to pursue the facility?
  - What are the current uses and capabilities of the facility?
  - Where are the capabilities going in the future and why (e.g. how did the 2013 BESAC report on the future of x-ray light sources factor into the revision of the LCLS-II project?)
  - What are representative examples of how the capability is supporting the basic research and applied research communities. Where possible, these examples are tied back to the science drivers described in chapters 4 through 9.

4. Understanding and Controlling Matter at the Atomic Scale, 4.1 X-ray Light Sources

- The five x-ray light sources stewarded by the Office of Science allow researchers to probe the interactions between photons, electrons, and chemical bonds, information necessary to understand, and ultimately control, the physical processes in the materials that are critical to the technologies described in the QTR.
- The wavelengths of the emitted photons span a range of dimensions, from the atom to biological cells, thereby providing incisive probes for research in materials science, physical and chemical sciences, metrology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences.
- The high brightness and penetrating ability of the x-rays allows researchers to study many energy systems while they are operating under realistic conditions.
- This section will survey the unique capabilities and applications of the five x-ray light sources:
  - *Storage ring sources*: Advanced Light Source (LBNL); Stanford Synchrotron Radiation Light Source (SLAC); National Synchrotron Light Source-II (BNL); Advanced Photon Source (ANL)
  - *Free Electron Lasers*: Linac Coherent Light Source (SLAC)





Source: (top) Advanced Photon Source, Argonne National Laboratory. (bottom) Linac Coherent Light Source, SLAC National Accelerator Laboratory.

4.2 Neutron Scattering

- The neutron scattering technique is well suited to the study of structural and dynamical properties in materials across a broad spectrum of scientific fields, including physics, biology, chemistry, polymer, engineering, and materials science.
- Neutrons are non-destructive and diffracted by materials, allowing for true 3D structural determinations without preference for light or heavy elements, which provides advantages for structural studies in soft matter and biological materials.
- This section will survey the unique capabilities and uses for the two neutron scattering facilities managed by the Office of Science:
    - Spallation Neutron Source, ORNL
    - High Flux Isotope Reactor, ORNL

(Top) Spallation neutron source. (Bottom) High Flux Isotope Reactor. Both facilities are located at Oak Ridge National Laboratory.

4.3 Nanoscale Science Research Centers

- *Nanoscience* is the study of materials and their behaviors at the nanometer scale. The scientific quest is to design new nanoscale materials and structures, and observe and understand how they function and interact with their environment.
- Developments at the nanoscale and mesoscale have the potential to deliver remarkable scientific discoveries that transform our understanding of energy and matter and advance national, economic, and energy security.
- The Office of Science supports five Nanoscale Science Research Centers (NSRC) as user facilities strategically located with other major facilities. The NSRCs complement one another with their instrumentation, capabilities, and expertise.
- This section surveys the unique capabilities and research programs of the five NSRCs:
  - Center for Functional Nanomaterials (BNL)
  - Center for Integrated Nanotechnologies (LANL & SNL)
  - Center for Nanoscale Materials (ANL)
  - Center for Nanophase Materials Science (ORNL)
  - The Molecular Foundry (LBNL)

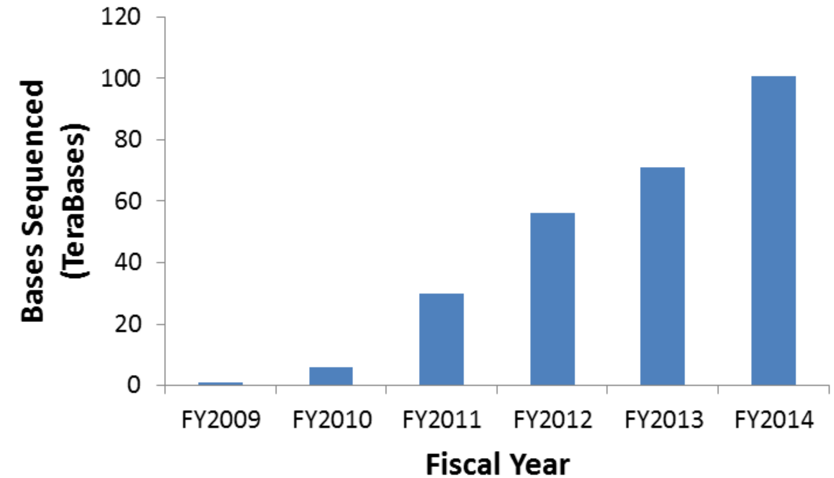
4.4 Environmental Molecular Science Laboratory

- The Environmental Molecular Science Laboratory (EMSL) leads molecular-level discoveries that are necessary to develop predictive, systems-level understanding for energy and environmental challenges.
- EMSL focuses on team-based research across four science themes – atmospheric aerosols, biological dynamics, subsurface and terrestrial ecosystems, and energy materials – and provides the experimental and theoretical capabilities that enable this science.
- This section surveys the approach to and character of the science mission, and the experimental and theoretical capabilities that support this effort. Selected near term developments in the facilities' capabilities are described.

4.5 Joint Genome Institute

- The Joint Genome Institute (JGI) is advancing genomics in support of the clean energy and environmental characterization missions of the DOE and BER program.
- JGI is developing high-throughput DNA sequencing and the computational and analytical tools necessary to manage the information (bottom right). This genomic information is the “source code” for biological structure and activity, and JGI provides a managed database and the tools needed to use it by the community.
- JGI works with the three BRCs to help identify the genes responsible for each step in the biofuel process, a critical step in controlling and ultimately improving biofuel production.
- This section surveys the enabling capabilities of the JGI, and describes their efforts in support of bioenergy and biofuels research. The JGI strategic planning practices and near term development goals are discussed.

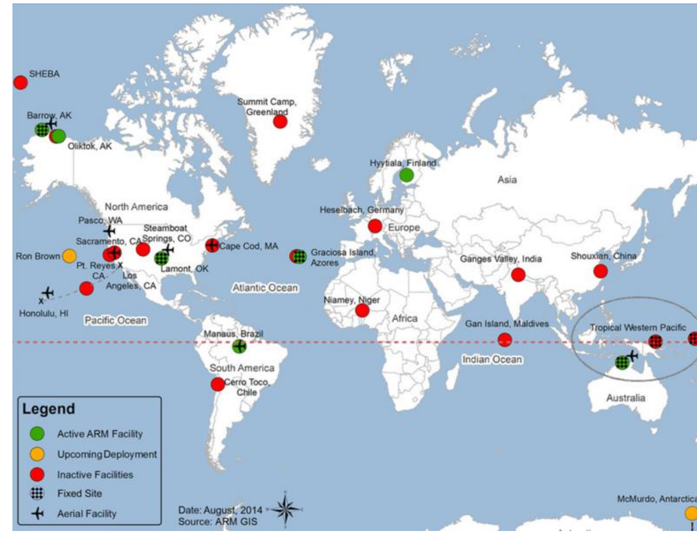
Source: Joint Genome Institute



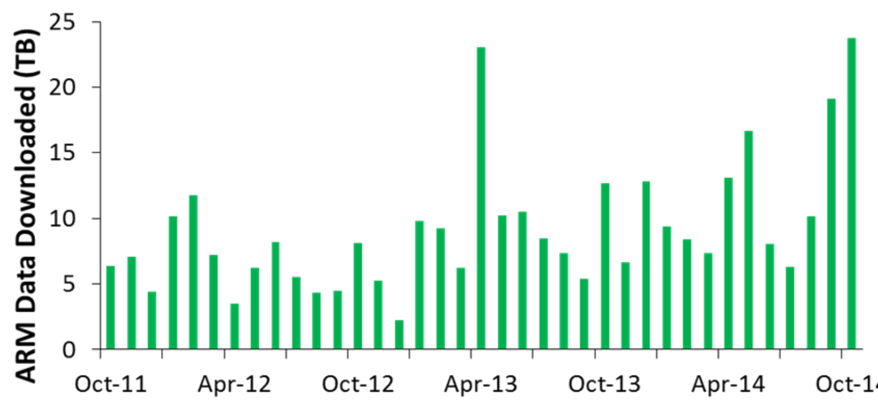
Source: Office of Biological and Environmental Research, Office of Science

4.6 Atmospheric Radiation Measurement Climate Research Facility

- The ARM Climate Research Facility is a user facility managed and operated by nine DOE laboratories. The ARM program manages a suite of facilities – fixed, mobile, and aerial - strategically located across the globe. Each facility utilizes state-of-the-art remote sensing and/or *in situ* instrumentation.
- The ARM program provides the climate research community with the tools and data necessary to improve climate and earth system models through better understanding of aerosols, clouds, and radiative transfer.
- This section surveys the capabilities of ARM, and provides examples for how the tools and data are improving a variety of climate models. Selected connections to the energy technology discussed in chapter 4-9 are included. Future efforts aimed at improving modeling and simulation capabilities and measurement density will be described.



ARM global facilities map for 2014. Source: Images, ARM Climate Research Facility (www.arm.gov)



Source: Office of Biological and Environmental Research, Office of Science

5. Modeling and Simulation of Complex Systems

- Simulation and modeling with advanced computing provides an opportunity to obtain insight into "how" a complex physical process works in ways not available through observation. This bridges the gap between well understood starting conditions and well characterized effects.
- The DOE is a leader in high performance computing – 15 of the fastest 150 computers are maintained by the DOE. As important as the hardware, DOE and ASCR are providing the tools needed to support application of these resources to basic research and applied research in support of all facets of the DOE mission.
- This section surveys existing DOE capabilities in three areas: computers, networking, and the algorithms, software, and personnel required to use the physical resources. Plans for increasing capabilities by reaching exascale performance, and the potential impact of exascale in applied technologies, is discussed.

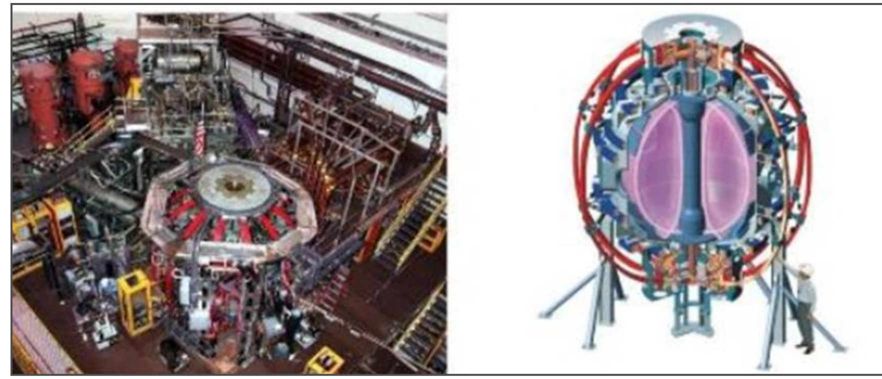
Leadership-class computing capabilities in the DOE. (Top) Titan (ORNL). (Bottom) Mira (ANL).

Technology Impacted	Project Title	Institution	Hours Allocated (Millions)
Batteries	Predictive Materials Modeling for Li-Air Battery Systems	Argonne National Laboratory	50
Fossil Fuels	Large-Eddy Simulation of the Bachalo-Johnson Flow, with Shock-Induced Separation	Boeing	135
Fusion	High-fidelity Simulation of Tokamak Edge Plasma Transport	Princeton Plasma Physics Laboratory	100
Hydrogen Energy	First-Principles Simulations of High-Speed Combustion and Detonation	University of Chicago	150
Nuclear	Nuclear Structure and Nuclear Reactions	Iowa University	100
Solar	Computational Spectroscopy of Heterogeneous Interfaces	University of Chicago	180

Selected 2015 INCITE projects with immediate relevance to energy technology. Source: Advanced Scientific Computing Research.

6. Fusion Science

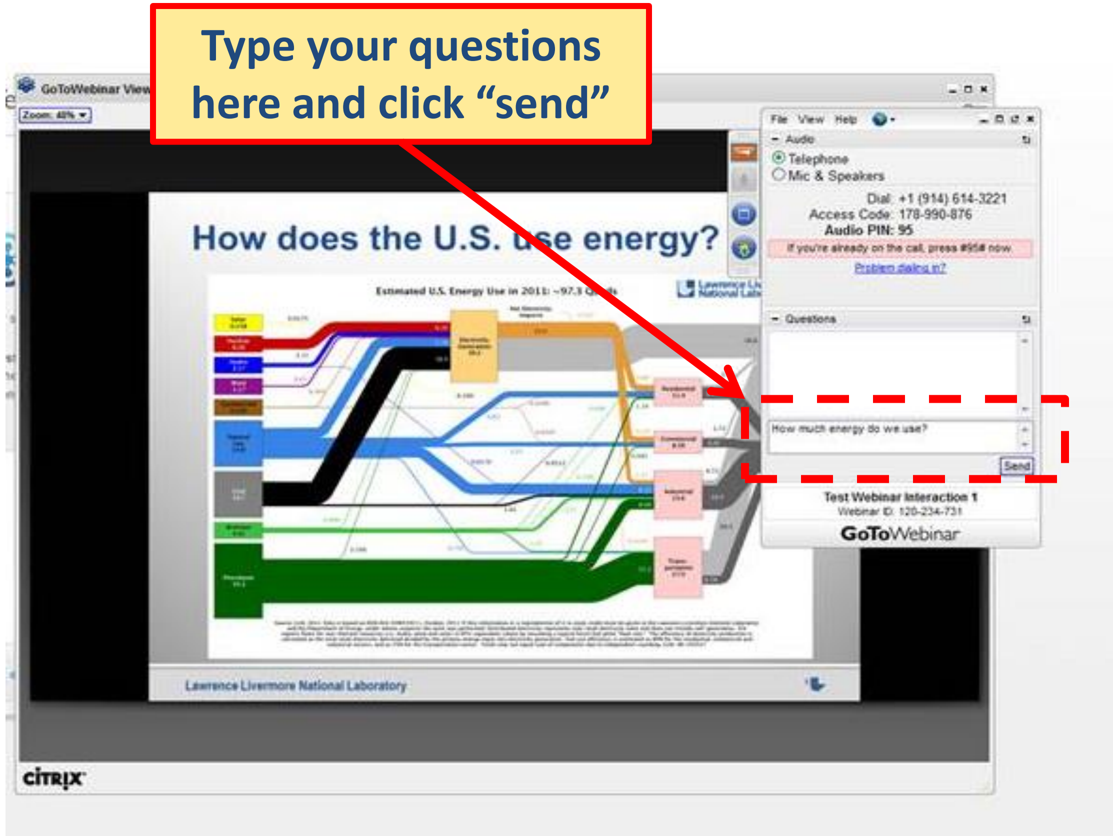
- Research in the Office of Fusion Energy Research (FES) is aimed at developing the fundamental scientific basis for a future fusion energy source.
- The basic science research program in FES is supported by two Office of Science User Facilities:
    - The National Spherical Torus Experiment (NSTX) (PPPL)
    - DIII-D (General Atomics)
- This section briefly describes the domestic user facilities, US participation in the ITER experiment, and some of the scientific challenges these programs are currently addressing.



(Top) the National Spherical Torus Experiment at Princeton Plasma Physics Laboratory. (Bottom) The inside of the DIIID Tokamak at General Atomics.

Public Input

- You are encouraged to submit questions using GoToWebinar’s “Questions” functionality. The moderators will respond, via audio broadcast, to as many appropriate questions as time allows.



- If you have questions or comments that cannot be addressed during the webinar, email them to DOE-QTR2015@hq.doe.gov

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