

U.S. Department of Energy

2016 SUMMARY REPORT DOE R&D CROSSCUTS January 2017

“The [Department of Energy’s FY 2017] budget request proposes several crosscutting initiatives that span several program offices. The Committee supports the Secretary’s efforts to reach outside of individual program offices to draw on the diverse disciplines within the agency as a whole. These initiatives...would allow for a more comprehensive review of complex issues. “

Senate Energy and Water Development Appropriations Bill, 2017, H.R. 2028, Committee Report 114-236, p. 58

This report summarizes the six U.S. Department of Energy (DOE) Research & Development (R&D)¹ Crosscuts. It provides a brief overview of the DOE Crosscut Team approach and describes the budget impact. The report includes a summary of the research focus areas for each of the six R&D Crosscut Teams.

I. PURPOSE, HISTORY, AND FUNCTION OF DOE’S CROSSCUT APPROACH

Purpose. Relentless innovation is the root of sustained success in the technology sector. To effectively pursue innovation in the United States energy system, the DOE must ensure that its R&D activities reflect the diversity and emerging challenges of the energy sector. While management of the broad DOE energy portfolio requires specialized expertise and a clear organizational structure, rich insights often derive from interdisciplinary idea formation and cross-organizational discussions.

The DOE’s R&D Crosscut Teams were established to formalize and enhance the coordination that has long-existed between the DOE science and energy program offices and the National Laboratories. Crosscut Teams serve as an information clearinghouse and expert exchange network, allowing the Department to rigorously examine and tackle many of the Nation’s largest energy-related R&D challenges. Importantly, the Crosscut Teams are charged with design of innovative new programs that stretch across organizational and budget boundaries. Leveraging the breadth of the DOE enterprise, the R&D Crosscut Teams reach across the Department to engage other, non-R&D DOE offices. Their efforts are also informed by consultation with external stakeholders from industry, academia, and state and local government entities. By creating these multi-office Crosscuts and putting funding on the table, the Department has created a network to incubate new approaches to program design and execution. The increased collaboration made possible through the Crosscut

¹ The Department also presents a Cybersecurity Crosscut each year as part of the DOE budget. The Cybersecurity Crosscut does not have an R&D focus, and, as a result, it is not discussed in this report.

Teams also enhances shared understanding of complementary activities and helps to avoid unintended overlap of investment across the energy innovation portfolio.

History. The Department reorganized in 2013, placing all of the science and applied energy programs under a single Under Secretary for Science and Energy. Leveraging this new structure and the linkages it enabled between the DOE's basic science and applied technology development programs, the Office of the Under Secretary for Science and Energy (US/SE) established six R&D Crosscut Teams in early 2014 to address high-priority research areas:

1. *Advanced Materials and Manufacturing*: supports coordinated R&D for advanced materials in multiple applications, including lightweighting and materials under extreme environments,²
2. *Energy-Water Nexus*: supports the Nation's transition to more resilient energy-water systems,
3. *Exascale Computing*: a joint Science-NNSA collaboration, significantly accelerates the development and deployment of next-generation high-performance computing systems,³
4. *Grid Modernization*: provides the tools to develop a resilient, secure, sustainable, reliable, flexible, and affordable grid of the future,
5. *Subsurface Science Technology, Engineering and Research*: enables mastery of the subsurface for a range of energy and environmental applications, and
6. *Supercritical Carbon Dioxide Technology*: develops a higher efficiency, lower water consumption, alternative power system for fossil, solar, and nuclear fueled electric power generation.

The DOE leadership identified these topics as areas with high potential impact for program offices across the DOE and for the external research and technology communities. Other areas of importance around which newer R&D teams are being formed include energy storage R&D and the development of efficient, interconnected urban systems. As teams like these work together to develop a proposed, coordinated R&D agenda, they have the potential to evolve into a formal crosscut through the budget process.

Function. During budget formulation, the R&D Crosscut Teams meet frequently to identify, analyze, and evaluate current and emerging research topics. Outside of the budget cycle, the teams continue to engage with external stakeholders. Maintaining this communication ensures that the Department's programs are implemented and executed in a manner that ensures maximum innovation potential for the Nation's benefit. The R&D Crosscut Teams also work throughout the year to:

- Establish common understanding of technical requirements, specifications, and terminology
- Analyze and evaluate new technologies and potential R&D pathways to advance them
- Develop broader strategy, planning and/or state-of-the-field science and energy reports
- Convene workshops/seminars and host regular information exchanges with internal and external experts (e.g. from the DOE's National Laboratories, industry, academia, etc.)

² The Advanced Materials and Manufacturing Crosscut Team was conceived and established in 2014 as part of the FY 2016 budget process. However, the resulting program was included for the first time in the FY 2017 budget as an "Advanced Materials" Crosscut.

³ In addition to the Exascale Crosscut Team, a related Advanced Computing Team works across the DOE programs and National Laboratories to facilitate improved understanding and increased use of high performance computing systems for energy sector applications.

- Draft or review Funding Opportunity Announcements (FOAs) of programs/offices participating in the Crosscut Team and cooperate on FOA merit reviews of submitted applications
- Coordinate program implementation activities, such as conducting joint analyses, joint FOAs, and shared student training programs to maximize individual Program investments

The US/SE routinely evaluates the R&D Crosscut Teams and may establish new teams or refocus or sun-set existing teams, where appropriate.

While all appropriated funds and program decisions ultimately reside with the separate offices involved in each Crosscut, the Department has found that programs are better able to identify and tackle common challenges when formulating budgets as an interdisciplinary team. In addition, the Crosscut Team structure has enabled more streamlined hand-offs from earlier stage and foundational research (e.g. in the DOE Office of Science) to more application-oriented technology development (in the DOE Applied Energy programs). Thus, the Crosscuts help to bridge the “valley of death” between lab-scale research and technology innovation.

II. CROSSCUT TEAM IMPACT

A simple yardstick to measure the success of the R&D Crosscuts is the amount of funding across all DOE programs that is now being coordinated through them. In FY 2016, the six R&D Crosscuts accounted for \$860 million, including funding in organizations ranging from the Office of Environmental Management to the National Nuclear Security Administration. The science and energy program portion of this total amounts to \$780 million, or about 16 percent of the DOE’s \$4.8 billion energy innovation portfolio.

The Crosscut concept has also received a positive reception from external stakeholders. For example, in both FY 2016 and FY 2017, the Committee Report of the Senate Energy and Water Development Appropriations Subcommittee included positive language in support of the Department’s Crosscut efforts. A passage from the FY 2017 report is included at the top of this report.

III. TECHNICAL/STRATEGIC CROSSCUT TEAM SNAPSHOTS

The latest budget figures for the six R&D Crosscut are detailed below, followed by one-page snapshots describing the purpose and major research areas for each.

Crosscut (\$ in M)	FY 2015 Current	FY 2016 Enacted	FY 2017 Request
Advanced Materials for Energy Innovation	42.7	48.0	113.5
Energy-Water Nexus	12.3	28.3	96.1
Exascale Computing Initiative	149.0	252.6	285.0
Grid Modernization	185.9	295.4	378.5
Subsurface Science, Technology, and Engineering R&D	164.7	207.2	258.3
Supercritical CO2	29.5	32.3	36.3
Total	584.1	863.8	1,167.7

Advanced Materials

Purpose

Affordable, reliable, high performance materials are key enablers to most transformational changes in technology, including critical clean energy applications. New materials discoveries have the potential to revolutionize whole industries, but only a small fraction of these materials make it to widespread market deployment. As a result, many new materials concepts that are hailed as scientific breakthroughs in the laboratory either never realize commercial application, or spend decades in the development cycle at significant cost. No matter how well a material performs in the laboratory, the uncertainties and risks associated with scale-up and production, as well as the real or perceived liabilities associated with material failures in service, significantly slow the pathway to deployment. To relieve this uncertainty and reduce risk, most sectors require that a new material be “qualified” before commercialization, invoking arduous and resource-intensive testing loops that can take years or even decades to complete.

The past decade has seen tremendous progress in tools development for materials research. The confluence of new theories, novel synthesis and characterization capabilities, and new computer platforms with the urgent demand for new energy technologies that require accelerated materials advancement at lower cost has created an unprecedented opportunity to impact the materials development cycle from scientific discovery to technological innovation. The Advanced Materials Crosscut is designed to accelerate the development of advanced materials for national security and energy applications, which is critical for U.S. manufacturing competitiveness in the 21st century.

Research Areas

A gap analysis comparing program priorities and current capabilities was conducted to determine where mutual opportunity space existed for both compelling new R&D and accelerated deployment of new advanced materials. Based on this assessment, two priority areas were identified for further investment:

Lightweight Materials & Composites – with emerging emphasis on polymer carbon fiber composites

Lightweight materials hold the potential for energy savings in energy generation, distribution and use. However, they can be costly, energy and carbon intensive and challenging to manufacture. Composite performance and energy intensity are limited by current polymer and reinforcement (e.g. carbon fibers) materials, for which new material discovery is required. Furthermore, the current process for manufacturing fibers, composites, and structures is also limited due to challenges in process scale-up.

Materials Under Extremes – with emerging emphasis on corrosion and extreme conditions

Corrosion can substantially reduce performance and useful lifetime and is estimated to cost 6% of the Gross Domestic Product (GDP), approaching 1 trillion per year.⁴ The 2015 Quadrennial Technology Review identified the manufacturing of materials for harsh service environments as a priority technical area for development, including materials for high-temperatures, pressures, radiation and chemical environments.

Additional potential focus areas for the future include semiconductors and quantum materials; chemical reactions and catalysis; energy conversion materials and devices; and critical materials.

⁴ *<http://www.g2mtlabs.com/2011/06/nace-cost-of-corrosion-study-update/>

Energy-Water Nexus

Purpose

Water and energy systems are interdependent, and several trends are increasing the urgency to address the energy-water nexus in an integrated way. First, precipitation and temperature patterns across the United States are undergoing rapid change with increasing frequency and intensity of extreme events. Record droughts, heat waves, floods, tropical storms, and winter storms have had significant effect on interdependent infrastructure, regional economies, and productivity in various parts of the U.S. Second, recent scientific evidence points to the accelerated drawdown of some critically important U.S. groundwater supplies, which typically serve as the “backup plan” for insufficient or intermittent surface water supplies for energy and other uses. Third, U.S. population growth and regional migration trends indicate that the population in arid areas such as the Southwest is likely to continue to increase, further impacting the management of both energy and water systems. Finally, introduction of new technologies in the energy and water domains could shift water and energy demands, potentially in disruptive ways if interdependencies are not explicitly addressed. The Energy-Water Nexus Crosscut builds on DOE’s 2014 *The Water Energy Nexus: Challenges and Opportunities* and is designed to assist the nation in moving towards more resilient and sustainable coupled energy-water systems.

Research Areas

Data, Modeling, and Analysis (DMA) - efforts will advance foundational models and integrate data sets to help decision-makers at Federal, regional, state, and municipal levels. Improving capabilities will provide insights into technology R&D opportunities. DMA work focuses on the following four sub-pillars:

- *Layered Energy Resilience Data-Knowledge System* will fill key data gaps, identify scope, prepare a preliminary design, and begin development of an integrated data analytic system.
- *Integrated Modeling Framework and Impact, Adaptation, and Vulnerability Model Development* will improve interoperability across a range of major modeling platforms that require integration to enable coupled simulations and predictive capabilities at the energy-water nexus.
- *Impacts, Adaptation, and Vulnerability Strategic Research and Analysis* will deliver a broad range of energy-water analyses, tools, and research insights.
- *Regional-Scale Data, Modeling, and Analysis Test Beds* will design and begin deployment of three regional-scale data, modeling, and analysis test beds.

Technology R&D - produces technology solutions to address vulnerabilities and increase resilience, and offers the possibility of efficiency improvements and cost reductions. R&D will focus on four sub-pillars:

- *A low-carbon, low-energy, low-cost desalination energy innovation hub* will serve as a center of research on enabling technologies for low-energy, low-cost desalination approaches that will support production of municipal drinking water, production of agricultural water supplies and treatment of nontraditional water sources, such as produced water from oil and gas extraction.
- *Energy-Optimized Treatment, Management, and Beneficial Use of Non-Traditional Water* will complement the hub, advancing targeted treatment technologies and low carbon energy sources to address treatment of non-traditional waters for projected beneficial uses.
- *Sustainable Low Energy Water Utilities* will pursue processes, technologies, and systems that increase efficiency and energy recovery in water and wastewater treatment and conveyance.
- *Water-Efficient Cooling for Electricity Generation* will pursue R&D on heat exchangers and cooling systems to reduce the need for water for cooling in thermoelectric power plants.

Policy Analysis and Stakeholder Engagement – informs understanding of the motivation and barriers for stakeholders addressing vulnerability and resilience of energy-water systems.

Exascale Computing

Purpose

The U.S. faces serious and urgent economic and national security threats. Over the past 20 years, high performance computing (HPC) has become essential for addressing such challenges for the Nation, and the development of the next generation of HPC is critical for solving these and future problems. In 2016, the Department established a high-priority goal to develop two diverse capable exascale systems - approximately 50 times the performance level of America's current fastest supercomputers - by the mid-2020s to address these challenges. U.S. government investment has been and will be critical.

Past partnerships between the U.S. government and computer industry have led to the development of highly innovative, beneficial technologies and the incorporation of them into product lines in ways that adherence to solely market forces would have precluded. Achieving a U.S. exascale computing capability requires a concerted national effort; within the Department, the Office of Science and the National Nuclear Security Administration are jointly leading this effort. Since the establishment of DOE's goal, China announced a new high performance computer built with solely Chinese components and software, which far exceeds the raw computational power of any U.S. HPC systems. Using that system, in November 2016 the Chinese scientists won the Gordon Bell prize for outstanding achievement in HPC, and that system occupies the #1 position on the 2016 June and November global TOP500 supercomputer lists. China currently has three exascale architecture designs in development and intends to deploy an advanced-architecture exascale system by 2020. Today the United States has a shrinking number of U.S. vendors, and failure to engage U.S. industry will open the door to China, which, with demonstrated commitment to immense HPC investment, will assume the leadership not only in high-end computing but eventually in national defense, science and energy technologies enabled by HPC - as well as in the commercial computing market. Addressing the threat that China poses to U.S. national and economic security requires acceleration of both hardware and software development, as well as related research. After analyzing the risks and opportunities afforded by acceleration of exascale computing, the Department significantly advanced its goal and directed the staged development of two capable exascale computing systems with advanced and diverse architectures by no later than 2021 and 2023.

Research Areas

The exascale development plan is organized around four technical focus areas:

Focus Area 1: Application Development

- Readiness to Utilize "Capable" Exascale Systems, initiating the development of a suite of national security, scientific, and engineering application software packages to ensure maximal impact of the exascale systems. This is achieved through co-design activities to support exploratory research between DOE National Laboratories and U.S. industry and universities, in both hardware and software areas.

Focus Area 2: Software Technology

- Software Technology Research and Development, aimed at developing the many necessary, complex exascale software technologies, including programming environments, scientific data management, software productivity and resilience, libraries and frameworks.

Focus Area 3: Hardware Technology

- Hardware Research and Development, to be conducted by U.S. computer vendors, aimed at developing exascale node and system architectures.

Focus Area 4: Exascale Systems

- Preparation for usable Exascale Systems, needed to support final advanced system engineering development and the acquisition and deployment of prototypes.

Grid Modernization

Purpose

Access to electricity is such a fundamental enabler for the economy that the National Academy of Engineering named “electrification” the greatest engineering achievement of the 20th century. However, the grid we have today does not have the attributes necessary to meet the demands of the 21st century and beyond. Five key trends are driving this transformation that challenges the capacity of the grid to provide us with the services we need, but also provides us with the opportunity to transform our grid into a platform for greater prosperity, growth, and innovation:

- Changing mix of types and characteristics of electric generation;
- Growing demands for a more resilient and reliable grid;
- Growing supply- and demand-side opportunities for customers to participate in electricity markets;
- Emergence of interconnected electricity information and control systems; and
- Aging electricity infrastructure.

The current business-as-usual trajectory for the electricity industry will not result in a timely transition to a modernized grid. Innovation in the electric power sector is inhibited by regulatory, market, and business model uncertainties. The Federal Government is in a unique position working with states, industry, and other stakeholders to accelerate efforts through research, development, and demonstration (RD&D), analysis, outreach, and convening initiatives. The Grid Modernization Crosscut focuses on developing the tools and technologies that measure, analyze, predict, protect, and control the grid of the future. In particular, DOE plays a significant role in:

- Cost-sharing R&D to accelerate the pace of technological innovation, especially where market fragmentation impedes the ability of individual entities to capture the value of investments.
- Providing solutions to unique regional issues to deliver collaborative partnerships and initiatives that are tailored to regional needs yet able to deliver national benefits.
- Overcoming information gaps and imperfections that otherwise cause market inefficiencies.
- Providing technical assistance to state entities to facilitate deployment of innovative grid technologies.
- Convening stakeholders in unbiased and meaningful dialogue on key issues.

Research Areas

The Grid Modernization Crosscut addresses three broad areas:

- *Technology*: Develop and demonstrate technologies for better measurement (e.g., sensors), integration (e.g., power electronics, energy storage, intelligent devices), management and control of grid operations (e.g., transformers, cyber-security).
- *Modeling and Analysis*: Develop and disseminate new and improved models for analysis, management, and optimization of grid performance (e.g., solar and wind prediction).
- *Institutional and Business*: Develop the analytical methodologies and frameworks for improving business models that can deliver to consumers the value and benefits of grid modernization.

An important new component of the Crosscut is a robust regional demonstration program to test and validate co-optimization across multiple grid attributes including affordability, security, resilience, reliability, and integration of innovative technologies.

Subsurface Science, Technology and Engineering R&D

Purpose

Energy sources originating from the Earth's subsurface constitute the Nation's primary source of energy, providing more than 80 percent of total United States energy needs. Discovering and effectively developing these resources, while mitigating impacts of their use, is critical to the Nation's secure, affordable, and sustainable energy future. The subsurface also provides safe storage capacity for carbon dioxide and other energy waste streams. Next-generation advances in subsurface technologies will:

- Enable prudent development of domestic oil and natural gas supplies
- Accelerate the deployment of sustainable fossil fuels by providing safe storage capacity for carbon
- Enable the deployment of up to 100GWe of geothermal energy
- Provide alternative disposal solutions for DOE-managed radioactive waste

Success in each of these areas requires mastery of the subsurface, including the ability to adaptively control subsurface fractures and fluid flow. The benefits of addressing this challenge now — increased safety, reliability, and competitiveness — are enormous.

Depressed oil and gas prices have recently led to a severe tightening of private industry R&D budgets⁵, with a loss of at least \$500M between 2013 and 2015. This has negatively impacted the pace of innovation, and the U.S. risks loss of its leadership position in the energy geosciences. The Subsurface Crosscut — including representatives from the Department's Nuclear, Fossil, Geothermal, Environmental Management and Basic Energy Sciences programs — is DOE's response to this challenge.

Research Areas

The Subsurface Crosscut is organized around four inter-related pillars for planning and implementing jointly-funded, targeted R&D and field demonstrations:

- *Wellbore Integrity* - The need to reduce the risk of uncontrolled release of formation fluid throughout the lifecycle of a wellbore extends across a wide range of geologic environments and time-scales. Well integrity is regarded as the single most important consideration for protecting groundwater resources that co-exist with energy production or storage operations.
- *Subsurface Stress & Induced Seismicity* - Knowledge of the subsurface stress state is required to predict and control the growth of hydraulically-induced fractures, re-opening of faults, and induced seismicity associated with completions, storage and waste disposal applications.
- *Permeability Manipulation & Fluid Control* - The current lack of precise control over fracturing and fluid flow despite decades of industrial practice is testimony to the huge challenges involved, primarily related to the difficulty of characterizing the deep subsurface and incomplete understanding of coupled subsurface processes.
- *New Subsurface Signals* - Due to the difficulty of characterizing the subsurface an entirely new class of capabilities is needed to characterize fractures and associated processes at sufficiently high spatial resolution and over large enough volumes to guide subsurface operations.

A critical component of all pillars will be R&D testing at Energy Field Observatories. Field tests are critical to the validation of new results and approaches at commercial scale to validate tools, technologies, and methodologies and measure progress.

⁵ Crooks, Ed. "Research cutbacks hit oil groups' ability to invest" < <https://www.ft.com/content/172d583c-1ab6-11e6-8fa5-44094fd9c46> > New York

Supercritical CO₂ Technology

Purpose

Power cycles that use supercritical carbon dioxide (sCO₂) as the working fluid have the potential to deliver significantly higher thermal efficiencies at lower cost than today's state-of-the-art, steam-based power plants. With successful development, the sCO₂ technology will make it possible to produce lower-cost electricity from diverse heat sources (e.g., coal, gas, nuclear, concentrated solar, or industrial waste heat) while simultaneously reducing emissions and water withdrawals. This technology also provides a far smaller physical footprint, enabling the required scalability and lower capital costs to facilitate distributed generation and improve regional energy security and resilience.

Steam-based stationary power generation provides 80% of the world's electricity, and the demonstrated fleet average efficiency is in the low-thirties, with the state of the art steam cycles averaging about 45%. Modeling of sCO₂ power cycles suggests the potential to reach efficiencies in excess of 50%, and the implications of a significantly more efficient power cycle are immense, representing billions of dollars in potential savings and a multi-billion dollar market. Given the capability of sCO₂ power cycles to take advantage of diverse heat sources and cost-efficiently convert them to usable power, novel applications may be expected. There is domestic and international interest for this technology to provide clean, affordable, and efficient shipboard power and propulsion. The DOE Fossil, Nuclear and Solar program offices have formed an sCO₂ Crosscut to overcome technical barriers and reduce risk to commercialization of the sCO₂ power cycle.

Research Areas

The sCO₂ crosscut is structured around a common objective to establish a 10 MWe Supercritical Transformational Electric Power (STEP) pilot scale facility by 2019 for evaluating power cycle and component performance over a range of operating conditions. Demonstrating favorable performance at this nominal scale is the next step required to address technical issues, reduce risk, and mature this promising technology. The 10 MWe facility is being cost-shared with industry and an award for its construction in San Antonio, TX was made in October 2016 through a competitive FOA selection process.

In tandem with the facility construction, R&D is being pursued on three major technical challenges:

- *Turbomachinery* - The high density, high pressure, and rapidly changing material properties of CO₂ near the critical point impose new challenges for turbomachinery design. High-quality designs and precision machining of both the compressor wheel and turbine wheel are essential to achieve high component and system efficiency. The sCO₂ design must provide sufficiently robust materials, seals, and blade cooling (for turbine inlet temperatures greater than nominal 1400°F [760 °C]) to account for differences in heat capacity, density, viscosity, and acoustic properties.
- *Recuperators* - Effective heat recuperation will significantly reduce the need for external heating and cooling energy. Major challenges are to optimize system design and balance increased recuperation with higher costs. A key objective is to avoid or reliably handle large pressure changes along the heat exchanger. Maturing manufacturing processes will be needed to improve the economics of diffusion-bonding techniques, investment-casting research, and in-service inspections.
- *Advanced Materials* - Novel materials will be needed to resist corrosion and erosion, carburization, creep, and fatigue under temperatures up to 1,300°F (750°C) and pressures up to 4500 psi (~300 bar). Material interactions can affect the design, reliability, and service lifetime of essentially all system components, and the long-term effects of various joining techniques (e.g., diffusion bonding, brazing) on corrosion rates require further study.