# Perspectives from the Office of Science

ASCAC Meeting
27 July 2015

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Acting Director, Office of Science

# Program Planning in SC

Mission Need

- Executive branch priorities
  - Administration priorities
    - National Science and Technology Council (and WGs)
    - Office of Science and Technology Policy (and WGs)
    - Other Administration convened ad hoc WGs
    - Interagency coordination
  - Departmental priorities
    - DOE and program strategic plans
    - Quadrennial Technology Review/Quadrennial Energy Review
- Congressional branch priorities
  - Legislative authorities and annual appropriations

Scientific Opportunity

- Program priorities, via engagement of community experts and stakeholders
  - Federal Advisory Committees*
  - DOE sponsored scientific and technical workshops/reports
  - Non-DOE (NRC, JASONS, …) sponsored scientific and technical workshops/reports

* *Virtually all major facilities and research programs in SC have roots in Federal Advisory Committee reports and recommendations.*

U.S. DEPARTMENT OF ENERGY

Office of the Under Secretary for Science and Energy

# Quadrennial Technology Review

Presentation to the
Basic Energy Sciences Advisory Committee


**Lynn Orr**
Under Secretary for Science and Energy


July 7, 2015

From S-4 @ BESAC

U.S. DEPARTMENT OF ENERGY

# QTR 2015 Chapter Outline

**Introduction**

1. National Energy System Strategic Objectives and Challenges
2. Energy Sectors and Systems

**Technology Assessments**

3. Enabling the Modernization of Electric Power Systems
4. Advancing Clean Electric Power Technologies
5. Increasing Efficiency of Building Systems and Technologies
6. Innovating Clean Energy Technologies in Advanced Manufacturing
7. Advancing Systems and Technologies to Produce Cleaner Fuels
8. Advancing Clean Transportation and Vehicle Systems and Technologies
9. Enabling Capabilities for Science and Energy RDD&D

**SC is here**

**Integrated Analysis**

10. Concepts in Integrated Analysis
11. Conclusions

12. Web Appendices

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# Tools for Scientific Discovery and Technology Development

- Investment in basic science research is expanding our understanding of how structure leads to function—from the atomic- and nanoscale to the mesoscale and beyond—in natural systems, and is enabling a transformation from observation to control and design of new systems with properties tailored to meet the requirements of the next generation of energy technologies.
- At the core of this new paradigm is a suite of experimental and computational tools that enable researchers to probe and manipulate matter at unprecedented resolution. The planning and development of these tools is rooted in basic science, but they are critically important for technology development, enabling discoveries that can lead to broad implementation.
- The challenges in energy science and technology development increasingly necessitate inter-disciplinary collaboration. The multi-disciplinary and multi-institutional research centers supported by the DOE are designed to integrate basic science and applied research to accelerate development of new and transformative energy technologies.
- These tools are available through a user facility model that provides merit-based open access for non-proprietary research. Eac[illegible]nds of users leverage the capabilities and staff expertise for their rese[illegible] expertise towards maintenance, developme[illegible]der com-

# Understanding and Controlling Matter at the Atomic Scale

***Unique, cutting-edge experimental tools for characterization, discovery, and synthesis of novel materials and energy systems.***

*X-ray light sources* provide a range of wavelengths capable of probing structures as small as atoms to whole cells and beyond.

- LCLS-II and APS-U will provide higher energy and brighter beams.
- Instrument development brings NSLS-II's world-leading beam brightness to more experiments.

*Neutron sources* are uniquely suited to non-destructive 3D structure determination of real systems.

- The SNS Second Target Station would enable new science in condensed matter, structural biology, and energy materials.

*Nanoscale Science Research Centers* integrate theory, synthesis, fabrication, and characterization of novel nanomaterials

- New capabilities in *in operando* electron microscopy and accelerator-based nanoscience.
- Novel fabrication techniques in combinatorics and self-assembly.

***On-going research, development, and upgrades for facilities opens new frontiers in materials characterization (real systems in real time).***

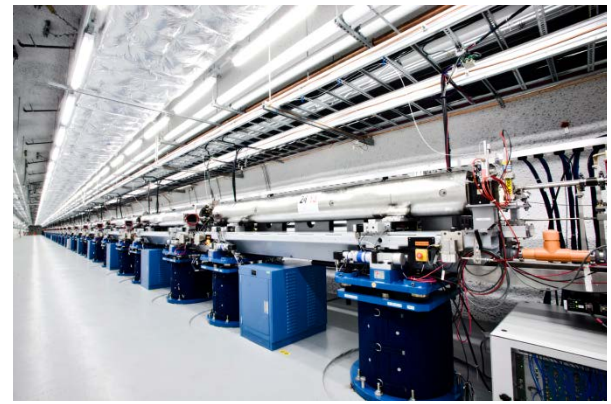
From S-4 @ BESAC

## Traversing a Catalytic Reaction Pathway in Femtosecond Steps

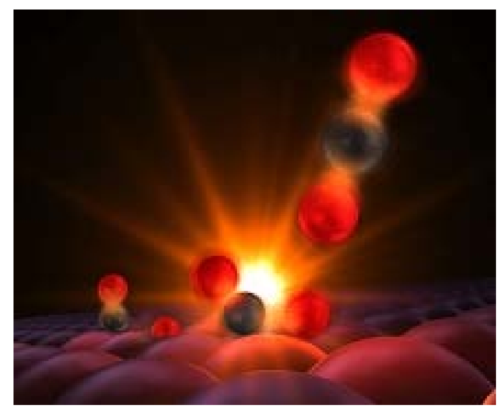
- SLAC researchers revealed details of a catalytic mechanism (CO oxidation at a ruthenium catalyst) by combining ultra-fast optical and x-ray laser pulses.

- Ultra-bright femtosecond x-ray pulses from LCLS allowed researchers to directly characterize catalytic reaction intermediates.

- The detailed understanding of elementary reaction steps enabled by LCLS opens the door for new catalysts that are both more reactive and more robust, leading to greater efficiency and reduced energy costs.



The 132 m LCLS undulator hall.



The stages of photoinitiated carbon monoxide oxidation at a ruthenium catalyst surface.

nce: Öström et al. "Probing the Transition State Region in CO Oxidation on Ru", *Science* **347**(6225), 978-982 (2015)

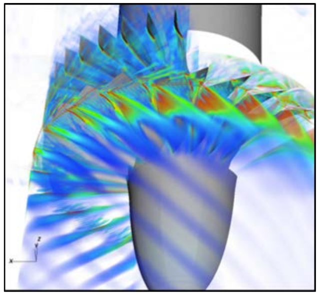
From S-4 @ BESAC

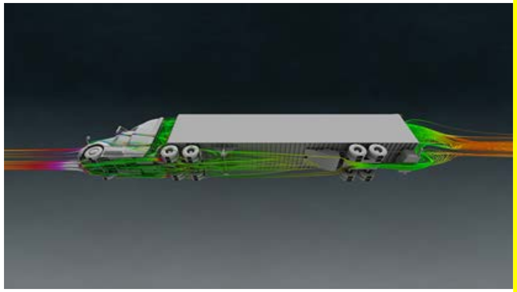
# Modeling and Simulation of Complex Phenomenon

***Accelerating discovery through modeling and simulation of real systems.***

- DOE and SC supported supercomputers enable simulation of complex real-world phenomena, putting true "systems-by-design" in reach.
- The *Office of Advanced Scientific Computing Research* supports this push to modeling and simulation of real systems through parallel development of hardware, software, and skilled personnel.
  - *Leadership-class computers*
  - *Production-class computers*
  - *Energy Sciences Network*
- DOE computers - enabled through dedicated outreach from the laboratories - have an enormous impact across the engineering and manufacturing space.
- The development needs of *exascale* computing – hardware, software, and efficiency – are being supported through *co-design* centers.

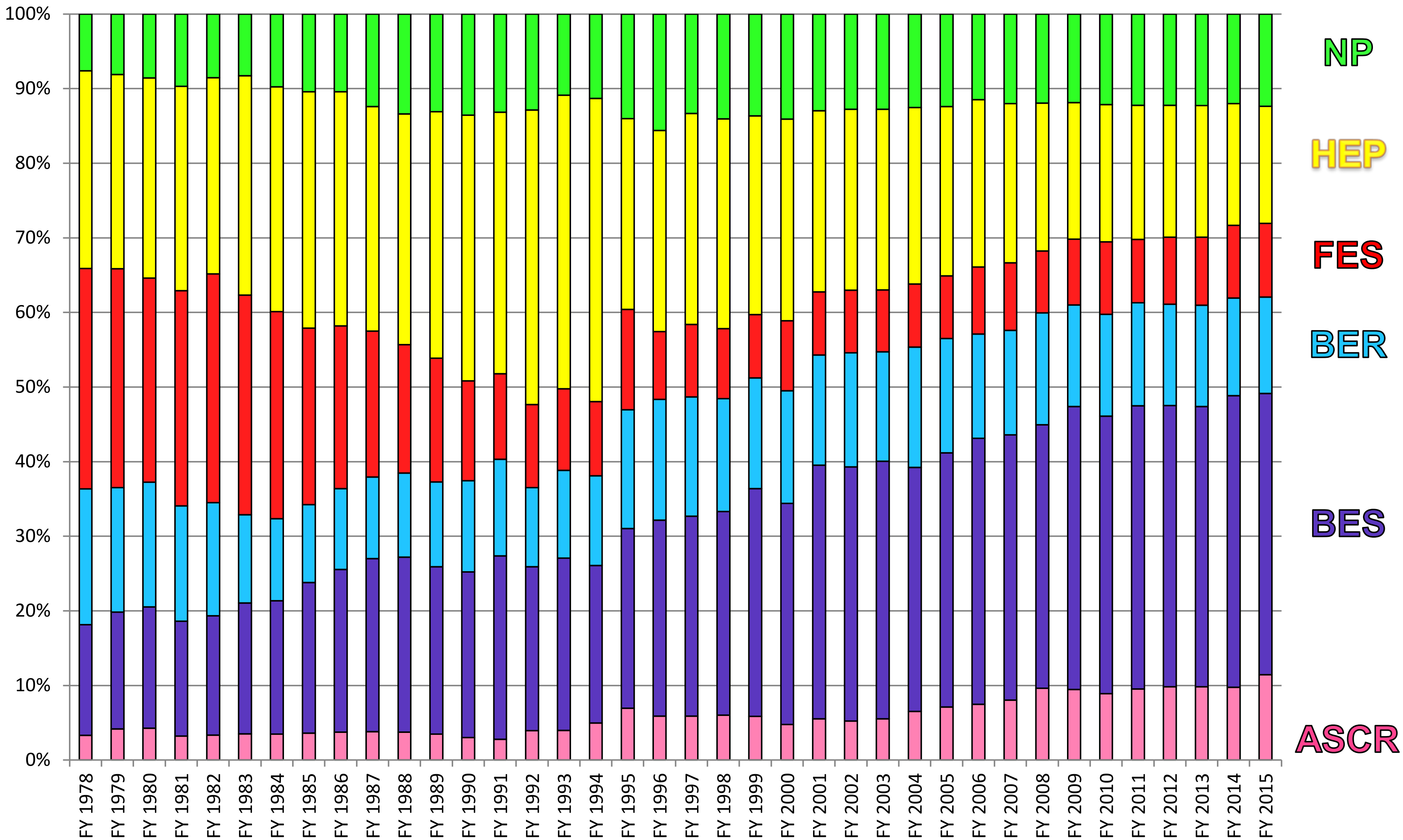
| Name | Performance (pflops/s) | Laboratory |
|---|---|---|
| Titan | 17.6 | Oak Ridge |
| Mira | 8.60 | Argonne |
| Cascade | 2.53 | Pacific Northwest |
| Edison | 1.65 | Lawrence Berkeley (NERSC) |
| Hopper | 1.05 | Lawrence Berkeley (NERSC) |
| Red Sky | 0.43 | Sandia/NREL |



From S-4 @ BESAC

# Major SC Program Funding (% of total) FY 1978-2015



# Charges/Reports: ASCAC, 2013-present

Excludes COVs and special topics, e.g., workforce development

1. **Determine potential synergies between the challenges of data-intensive science and exascale computing.** (Charge given July 25, 2012; *"Synergistic Challenges in Data-Intensive Science and Exascale Computing"* delivered March 2013).

2. **Determine the 10 principal research challenges and the technical approaches (hardware and software) required to develop a practical exascale computing system.** (Charge given July 29, 2013; *"The Top Ten Exascale Research Challenges"* delivered February 10, 2014).

3. **Review the Department's draft preliminary conceptual design for the Exascale Computing Initiative.** Specifically, determine whether there are gaps in DOE's plans or areas that need to be given priority or extra management attention. (Charge given November 19, 2014; preliminary report due March 30, 2015; final report due September 30, 2015).

# Charges/Reports: BESAC, 2013-present

Excludes COVs and special topics, e.g., workforce development

1. **Provide advice on the future of photon sources and science, considering both new science opportunities and new photon source technologies in parallel.**
   - Assessment of the grand science challenges that could best be explored with current and possible future SC light sources. The assessment should cover the disciplines supported by Basic Energy Sciences (BES) and other fields that benefit from intense light sources.
   - Evaluation of the effectiveness of the present SC light source portfolio to meet these grand science challenges.
   - Enumeration of future light source performance specifications that would maximize the impact on grand science challenges.
   - Prioritized recommendations on which future light source concepts and the technology behind them are best suited to achieve these performance specifications.
   - Identification of prioritized research and development initiatives to accelerate the realization of these future light source facilities in a cost effective manner.

   (Charge given January 2, 2013; *"Report of the BESAC Subcommittee on Future X-ray Light Sources"* delivered July 25, 2013).

2. **Revisit the BESAC 2007 "Challenges" Report (*"Five Challenges for Science and the Imagination"*) considering progress achieved, impact of the challenges on energy sciences, funding modalities, and new areas of basic research not described in the original report.** (Charge given February 11, 2014; report requested in 2015.)

# Charges/Reports: BERAC, 2013-present

Excludes COVs and special topics, e.g., workforce development

1. **Recommend initiatives for field-based research (the so-called Integrated Field Laboratory) that capture a multi-disciplinary approach and build on observations and modeling: (1) define the criteria for selecting sites for future BER field-based research and (2) prioritize the sites identified or described.** As described by BERAC in 2013, the IFLs are highly instrumented laboratories that build on existing BER observational and modeling capabilities that serve to integrate and expand vertically (from the bedrock to the atmosphere) and geographically (across key geographic regions).

   (Charge given September 23, 2014; draft report presented February 19, 2015; final report due fall 2015. This charge continues earlier BERAC charges that resulted in: *"Grand Challenges for Biological and Environmental Research: A Long-Term Vision"* December 2010; *"BER Virtual Laboratory: Innovative Framework for Biological and Environmental Grand Challenges"* February 2013)

# Charges/Reports: FESAC, 2013-present

Excludes COVs and special topics, e.g., workforce development

1. **Assess priorities among and within the elements of the magnetic fusion energy science program.** (Charge given April 13, 2012; "Report of the FESAC Subcommittee on the Priorities of the Magnetic Fusion Energy Science Program" delivered March 2013).

2. **Develop a strategic plan for the Fusion Energy Sciences program** assuming several different funding scenarios that will ensure long-term U.S. leadership in the foundations of burning plasma science (the science of prediction and control of burning plasmas); long-pulse burning plasma science (the science of fusion plasmas and materials approaching and beyond ITER); and discovery plasma science (the science of laboratory plasmas and the high energy density state). (Charge given April 8, 2014; *"Report on Strategic Planning: Priorities Assessment and Budget Scenarios"* delivered December 2014).

3. **Assess connections between research supported by the Fusion Energy Sciences program and other scientific disciplines and technological applications.** (Charge given February 4, 2015; report requested in 2015.)

# Charges/Reports: HEPAP, 2013-present

Excludes COVs and special topics, e.g., workforce development

1. **HEPAP via the P5 panel (i.e, the Particle Physics Project Prioritization Panel) should develop an updated strategic plan for U.S. high energy physics that can be executed over a 10-year timescale in the context of a 20-year global vision for the field.** Consider the recent discovery of the long-sought Higgs boson, the observation of missing among all three known neutrino types at unexpectedly large rates, and budgets that are more stringent than those considered by the previous P5 panel (2008). (Charge given September 2013; *"Building for Discovery: Strategic Plan for U.S. Particle Physics in the Global Context"* delivered May 22, 2014.)

2. **Assess the accelerator R&D effort supported by the High Energy Physics program.** (Charge given June 10, 2014; *"Accelerating Discovery: A Strategic Plan for Accelerator R&D in the U.S."* delivered May 18, 2015.)

# Charges/Reports: NSAC, 2013-present

Excludes COVs and special topics, e.g., workforce development

1. **Provide advice for an effective strategy for implementing a possible 2nd generation U.S. experiment on Neutrinoless Double Beta Decay (NLDBD) capable of reaching the sensitivity necessary to determine whether the neutrino is a Majorana or Dirac particle.** (Charge given December 2013; *"Report to* NSAC on Neutrinoless Double Beta Decay" delivered April 24, 2014.)

2. **Conduct a new study of the opportunities and priorities for U.S. nuclear physics research, and recommend a long-range plan that will provide a framework for coordinated advancement for the nation's nuclear science research programs over the next decade.** (Charge given April 23, 2014; report requested October 2015.)

3. **Establish an NSAC Isotope (NSACI) subcommittee for an initial period of two years to conduct a new study of the opportunities and priorities for isotope research and production, an effort that should result in a long-range strategic plan for the DOE Isotope Program managed by the Nuclear Physics program.** (Charge given April 23, 2014; report requested March 2015.)

4. **Provide additional advice for an effective strategy for implementing a possible 2nd generation U.S. experiment on Neutrinoless Double Beta Decay (NLDBD) capable of reaching the sensitivity necessary to determine whether the neutrino is a Majorana or Dirac particle under the inverted-hierarchy mass scenario.** (Charge given March 30, 2015; report requested November 2015.)

# Office of Science FY 2016 Budget Request to Congress

(Dollars in thousands)

| | FY 2015 | | FY 2016 | | |
|---|---|---|---|---|---|
| | President's Request | Enacted Approp. | President's Request | House Mark | Senate Mark |
| SCIENCE | | | | | |
| Advanced Scientific Computing Research.................................. | 541,000 | 541,000 | 620,994 | 537,539 | 620,994 |
| Basic Energy Sciences........................................................... | 1,806,500 | 1,733,200 | 1,849,300 | 1,770,306 | 1,844,300 |
| Biological and Environmental Research.................................... | 628,000 | 592,000 | 612,400 | 538,000 | 610,000 |
| Fusion Energy Sciences.......................................................... | 416,000 | 467,500 | 420,000 | 467,600 | 270,168 |
| High Energy Physics............................................................... | 744,000 | 766,000 | 788,000 | 776,000 | 788,100 |
| Nuclear Physics...................................................................... | 593,573 | 595,500 | 624,600 | 616,165 | 591,500 |
| Workforce Development for Teachers and Scientists................ | 19,500 | 19,500 | 20,500 | 20,500 | 19,500 |
| Science Laboratory Infrastructure........................................... | 79,189 | 79,600 | 113,600 | 89,890 | 113,600 |
| Safeguards and Security......................................................... | 94,000 | 93,000 | 103,000 | 103,000 | 100,715 |
| Program Direction.................................................................. | 189,393 | 183,700 | 187,400 | 181,000 | 185,000 |
| Subtotal, Science.................................................................. | 5,111,155 | 5,071,000 | 5,339,794 | 5,100,000 | 5,143,877 |
| Rescission of Prior Year Balances............................................ | ...... | -3,262 | ...... | -4,717 | -4,717 |
| Total, Science Approp........................................................... | 5,111,155 | 5,067,738 | 5,339,794 | 5,095,283 | 5,139,160 |