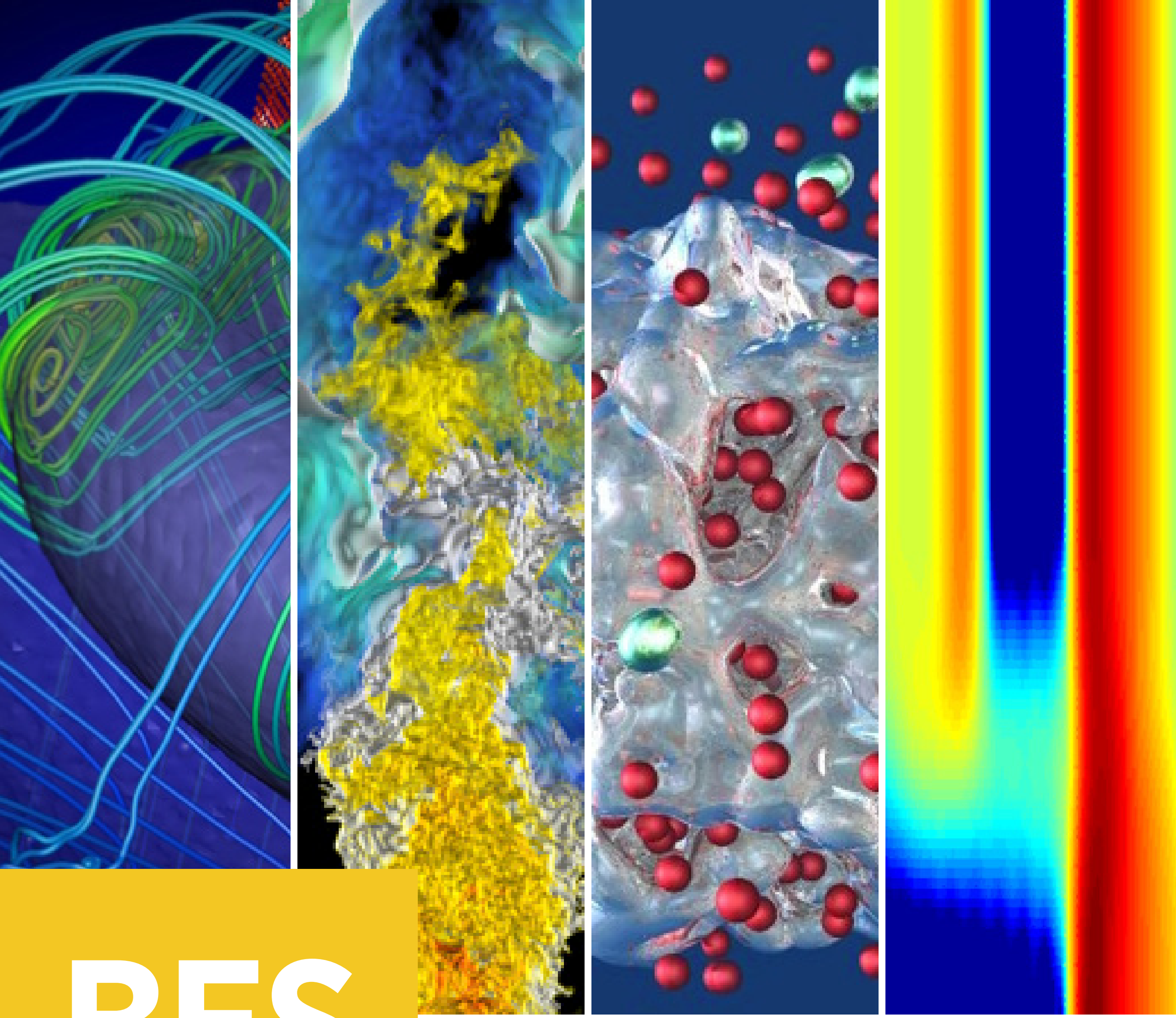

BES

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by
Advanced Scientific Computing Research
and Basic Energy Sciences

November 3–5, 2015
Rockville, Maryland

U.S. DEPARTMENT OF ENERGY

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1
YEAR OF **PLANNING**

3
DAYS OF **DISCUSSION**

36
WHITE PAPERS AND

21
CASE STUDIES PREPARED IN ADVANCE OF THE REVIEW

100
PARTICIPANTS FROM MORE THAN 40 **INSTITUTIONS**

Exascale Requirements Reviews: Overview

During 2015 and 2016, the U.S. Department of Energy (DOE) conducted Exascale Requirements Reviews for each of its six Office of Science (SC) program offices. The goal of the reviews was to help ensure the ability of DOE's Advanced Scientific Computing Research (ASCR) facilities to support SC mission science in the exascale age. The reviews brought together scientists, planners, and experts to identify:

1. **Grand Challenges:** forefront scientific challenges and opportunities that could benefit from exascale computing over the next decade.
2. **Priority Research Directions:** how new high-performance computing (HPC) capabilities will be used to advance boundaries at the various scientific frontiers.
3. **Computing Requirements:** how to maximize the potential for exascale computing to advance scientific discovery and understanding.

DOE program managers are using the review reports to guide strategic planning and investments for the 2017–2025 time frame.

BES Grand Challenges

For its Exascale Requirements Review, Basic Energy Sciences (BES) made use of five grand challenges developed in 2015 to inspire and guide BES research.

New Themes

1. Mastering hierarchical architectures and beyond-equilibrium matter.
2. Beyond ideal material and chemical systems: understanding the critical roles of heterogeneity, interfaces, and disorder.
3. Harnessing coherence in light and matter.

Cross-Cutting Opportunities

4. Exploiting transformative advances in imaging capabilities across multiple scales.
5. Achieving revolutionary advances in models, mathematics, algorithms, data, and computing.

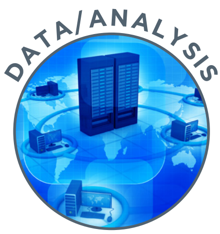
Addressing these challenges would spark revolutionary scientific advances for changes that meet some of the most pressing energy needs.

Strong connections must exist among advanced theoretical/algorithmic developments, new computing landscapes, and experimental toolsets.

Answering BES Challenges in the Exascale Age

Participants at the BES review identified these broadly grouped findings that would directly affect the BES mission need:

- Theory, simulation, visualization, and data analysis are crucial for advances in energy science.
- Revolutionary mathematical, software, and algorithm developments are required in all areas of BES science to take advantage of exascale computing architectures and to meet data analysis, management, and workflow needs.
- In partnership with ASCR, BES has an emerging and pressing need to develop new and disruptive capabilities in data science.
- More capable and larger high-performance computing and data ecosystems are required to support priority research in BES.
- Continued success in BES research requires developing the next-generation workforce through education and training and by providing sustained career opportunities.



BES Priority Research Directions and Computing Needs

The BES Exascale Requirements Review focused on eight areas for which an exascale ecosystem can be transformative.

Novel Quantum Materials and Chemicals

Future energy technologies will rely on specific combinations of elements, materials, and phases whose behaviors are “emergent” or not predictable by studying their components in isolation. Developing new, predictive theories and efficient and adaptive software and exploiting the full capabilities of new and future computing architectures at BES/ASCR facilities are critical to designing chemicals and materials with desired emergent properties.

Catalysis, Photosynthesis and Light Harvesting, and Combustion

Understanding and controlling chemical transformations and energy conversion are core to the BES mission. Current computational limitations severely restrict the size and complexity of systems that can be studied with sufficient fidelity. Emerging computing ecosystems, along with advances in theoretical methods and algorithms, will enable study of realistic heterogeneous environments at long time and length scales, significantly enhancing prediction reliability.

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Materials and Chemical Discovery

The biggest challenges to realizing the vision of materials and chemical discovery "by design" are predicting novel materials and chemicals with targeted properties and creating corresponding synthesis and degradation pathways. Progress will require advances in theory, predictive modeling capabilities, hardware resources, and experimental techniques to migrate to an adaptive, multiscale modeling paradigm.

Soft Matter

The complexity of soft matter — polymers, liquids, gels, or amorphous solids, etc. — presents scientific as well as computational challenges in designing functional matter for applications in energy storage and production, chemical separations, enhanced oil recovery, food packaging, chip manufacturing, and health care. Researchers expect to access many interesting phenomena in soft matter with exascale resources, enabling modeling that will have a significant and broader impact on critical national needs.

Advances in Algorithms for Quantum Systems

While advances in quantum and multiscale methods affect computational chemistry, biology, physics, and materials science, the associated high computational cost of scaling poses significant challenges. Facilitating use of these methods will involve reducing the scaling and developing multilevel parallel algorithms for them, requiring collaboration among application scientists and developers, applied mathematicians, computer scientists, and software engineers.

Computing and Data Challenges at BES Facilities

The BES program operates major scientific user facilities where more than 240 different types of instruments require complex data acquisition and analysis methods. Future facilities will support expanded instrumentation and techniques, leading to an exponential growth in data. Managing and extracting useful scientific information from these data, combined with real-time modeling and simulations during the experiments, will require exascale computational resources.

Mathematics and Computer Science Transforming BES Science

Bridging the gap between BES scientific goals and ASCR computing capabilities will depend on the collective abilities of the science domains and facilities to deliver breakthroughs in mathematics and computer science. These needs include improvements in speed and accuracy in predictive modeling; algorithms and software environments for fast, multimodal analysis of multisource data; and tools that make the efficient programming of tomorrow's machines as straightforward as programming today's laptops.

Next-Generation Workforce

Fielding a sufficiently skilled workforce is a major challenge in realizing exascale computational science. Significant investments must be made in training a new generation of scientists who are well grounded not only in their technical disciplines, but who are also knowledgeable about relevant computer science and applied mathematics issues.

The Exascale Requirements Review reports and supporting materials can be found at http://exascaleage.org

DOE's HPC centers are based at Argonne National Laboratory (ALCF), Lawrence Berkeley National Laboratory (NERSC), and Oak Ridge National Laboratory (OLCF), with networking services provided by ESNet; all of these facilities operate under the direction of ASCR.

Argonne NATIONAL LABORATORY · ESnet ENERGY SCIENCES NETWORK · NERSC · OAK RIDGE National Laboratory