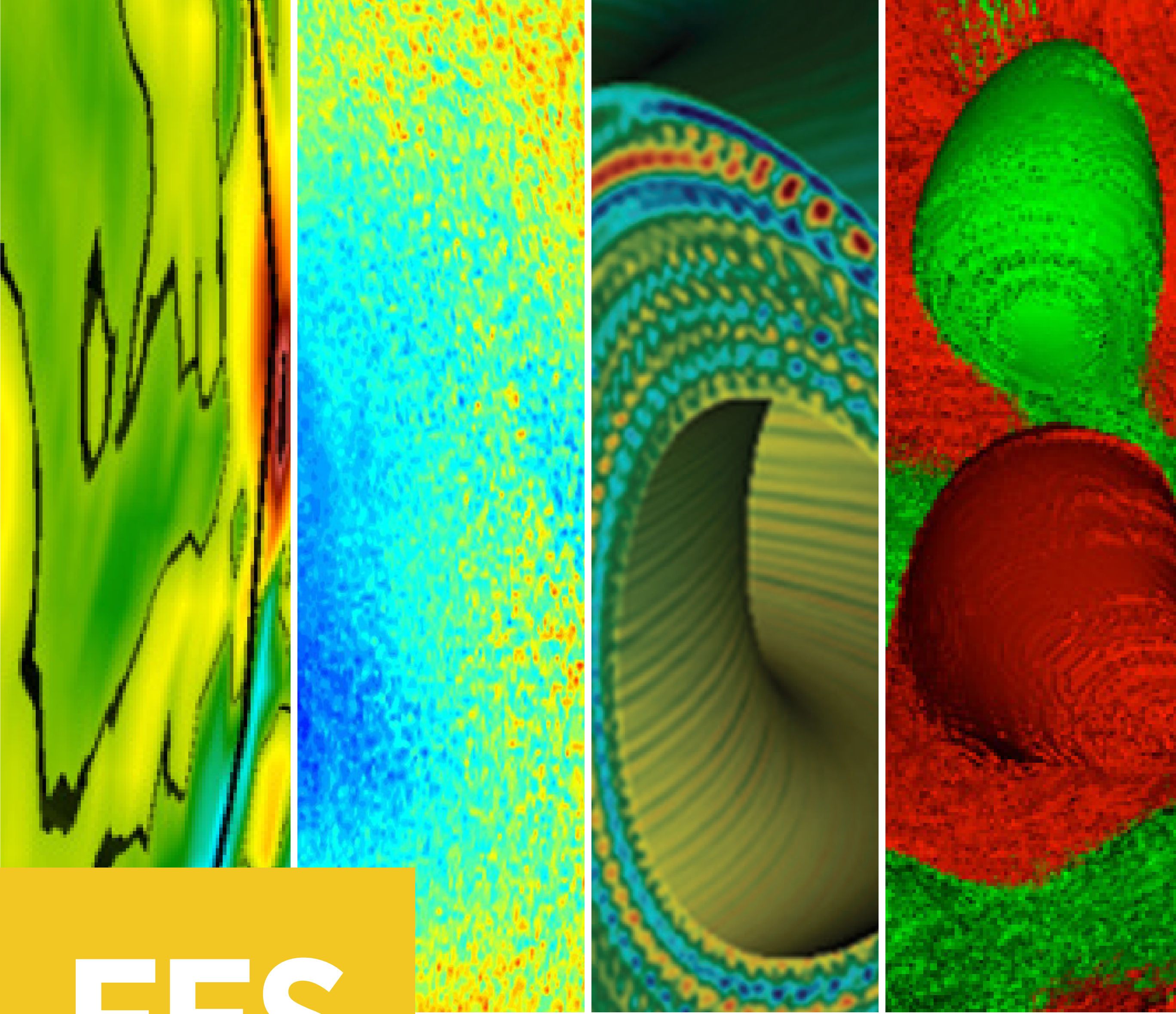

FES

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EXASCALE REQUIREMENTS REVIEW

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1
YEAR OF **PLANNING**

3
DAYS OF DISCUSSION

33
WHITE PAPERS AND **CASE STUDIES** PREPARED IN ADVANCE OF THE REVIEW

100
PARTICIPANTS FROM MORE THAN 35 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.

DOE program managers are using the review reports to guide strategic planning and investments for the 2020–2025 time frame.

FES Grand Challenges

In its 2015 ten-year strategic plan, Fusion Energy Sciences (FES) highlighted five areas of critical importance for the U.S. fusion sciences program:

– Massively parallel computing to validate modeling of whole fusion devices, enable transformative predictive power, and thus minimize risk in future development steps.
– Materials science as it relates to plasma and fusion sciences to provide the scientific foundations for greatly improved plasma confinement and heat exhaust.
– Research to predict and control transient events and thus address deleterious impacts on toroidal fusion plasma confinement and enhance machine designs and operation with stable plasmas.
– Continued stewardship of discovery in plasma science to address great mysteries of the visible universe and attract and retain a new generation of plasma/fusion science leaders.
– FES user facilities to keep world-leading through robust operations support and regular upgrades.

Strong connections must exist between advanced theoretical/algorithmic developments, new computing landscapes, and experimental toolsets to realize these transformational opportunities.

Answering FES Challenges in the Exascale Age

Participants at the FES Exascale Requirements Review identified these broadly grouped findings that would directly affect the FES mission need:

- Progress in computation across the range of fusion and plasma topics in recent years has been dramatic. Advances can be attributed to coordinated improvements in theory, computational and mathematical algorithms, performance engineering, computing hardware and software platforms, and uncertainty quantification (UQ).
- Broader and deeper integration into multiphysics and multiscale domains is a critical next step and will be necessary to address many important questions. These are exascale-level problems. Dramatically increased computing needs are also driven by ensemble runs in support of uncertainty quantification.
- The technical implementations for practical and affordable exascale platforms will present a number of significant challenges to approaches and algorithms used in today's codes. Additional challenges are presented in the areas of fault tolerance, software engineering, workflows, data management, in-situ analytics, and visualization.
- Close collaboration among stakeholders in various communities will be crucial to overcoming these challenges and realizing the advantages afforded by the new platforms. To that end, a large and specific set of needs for improved computational techniques, programming models, tools, software libraries, and algorithms have been identified.
- Predictable and stable access to high-performance computing resources is essential if the returns from major programmatic investments in code development are to be realized. In general, closer integration of processes for funding people and projects on the one hand and provisioning computer time on the other could lead to more efficient and optimal outcomes.

Priority Research Directions

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

Fusion Energy Science

Turbulence and Transport in a Fusion Reactor

Plasma turbulence and transport determine the viability of a fusion reactor: if plasma energy is lost too quickly, fusion burn cannot occur or be sustained, and core confinement will not be realized if plasma is not confined at the edge. Running well-resolved, full-torus gyrokinetic simulations for ITER and fusion reactors will require exascale-class supercomputers to obtain reliable prediction of radial temperature and density profiles Turbulence and transport simulations in the core and edge regions at exascale will set up the basis for other priority fusion science areas.

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Energetic Particles and Magnetohydrodynamic Instabilities in a Fusion Reactor

Energetic particles (EPs) in burning plasma experiments can readily excite macroscopic magnetohydrodynamic (MHD) instabilities, which, in addition to other mechanisms, can lead to disruptions or threaten a machine's integrity. Predictive capability requires exascale-level, integrated first-principles simulation of nonlinear interactions of multiple kinetic-MHD processes.

RF Heating in a Fusion Reactor

The robust and efficient application of high-power radio frequency (RF) systems is critical in the ion cyclotron, electron cyclotron, and lower hybrid ranges of frequencies, necessitating fidelity in modeling how RF waves interact with the tenuous edge plasma of a fusion device. Emerging exascale architectures would enable models that fully account for the multiscale and multiphysics nature of RF heating and current drive.

Whole-Device Fusion Modeling

In the hot fusion plasma in a toroidal geometry, several multiphysics processes, as described here, are working together; most are scale inseparable and interacting nonlinearly in a self-organized manner. A whole-device modeling approach is needed to understand and predict the fusion reactor plasma. This effort cannot be realized without exascale (or beyond) computational capability at high fidelity.

Plasma Surface Interactions and Structural Materials

Developing first-wall material and component solutions for future fusion devices (ITER, DEMO) is prohibitively costly, necessitating a multiscale modeling approach. An integrated and first-principles-based suite of advanced codes will be needed to model the boundary plasma and material surface.

Discovery Plasma Science

General Plasma Science

Modeling plasma turbulence remains beyond the capabilities of today's most advanced computers and algorithms. Exascale computing will enable direct numerical simulations of the high-dimensional, nonlinear turbulent dynamics.

High-Energy-Density Laboratory Plasmas

HEDLPs are extreme states of matter having pressures in excess of 1 Megabar. The physics of laser-plasma interactions and HEDLPs is multiscale, highly nonlinear, and must often be described by a kinetic modeling approach. Extreme HPC resources will enable increasing the problem size and grid resolution, running ensembles, and reducing turnover time.

Low-Temperature Plasmas

LTPs are partially ionized gases involved in the manufacture of electronics components and are typically in a strongly nonequilibrium state. Providing high-confidence models will transform the applied use of LTPs in industry.

Verification, Validation, and Uncertainty Quantification

Confidence in "validated predictive models" must be earned through systematic confrontation with experimental data and a sharp focus on careful and quantitative estimates of errors and uncertainties. New methodologies and algorithms must address mathematical obstacles in multiphysics integration and use of computationally expensive codes in multiscale integration.

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.