U.S. DEPARTMENT OF ENERGY | Office of Science

ASCR Requirements Review

ASCR Program Office Summary
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For presentation to the BER Advisory Committee

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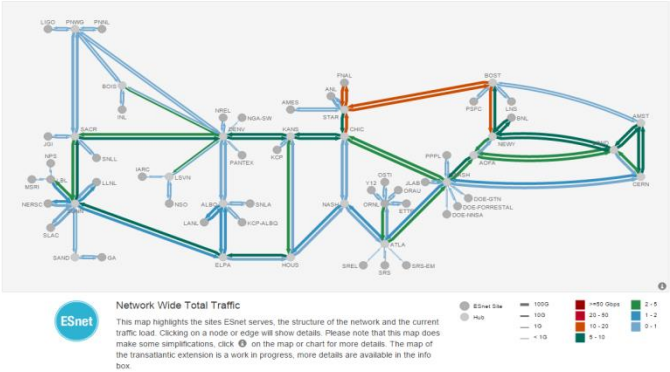
October 27, 2016

ASCR's Facilities

Providing the Facilities – **High-End and Leadership Computing**

- **National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory**
  - Delivers high-end capacity computing to entire DOE SC research community
  - Over 6,000 users and 800 projects
- **Leadership Computing Centers at Argonne National Laboratory (ALCF) and Oak Ridge National Laboratory (OLCF)**
  - Delivers highest computational capability
    - Open to national and international researchers, including industry
    - Not constrained by existing DOE or Office of Science funding or topic areas
  - Approximately 1,000 users and 50-60 projects at each center, each year



Linking it all together – **Energy Sciences Network (ESnet)**

Path to the Future – **Research & Evaluation Prototypes**

Previous Requirements Gathering Efforts: "Lead with the Science"

Value of Approach

- **Review meetings establish consensus on requirements, capabilities, services**
- **Scientists, programs offices, and facilities have the same conversation**
- **Provides a solid, fact-based foundation for service and capability investments**
- **Addresses DOE mission goals by ensuring DOE science is effectively supported**

Requirements Reviews Need to Meet Multiple Needs

- **Facilities needs**
  - Develop mission need statements for proposed upgrades
  - Identify emerging hardware and software needs of researchers, including experimentalists at SC or other scientific user facilities or experiments
- **Headquarters needs**
  - Articulate the case for future upgrades to SC and DOE management, OMB and Congress
    - What are the potential impacts from the investments in upgrades
    - How broad is the reach – industry, other user facilities, other agencies
  - Identify emerging hardware and software needs for SC, including research
    - What gaps can we fill
  - Develop strategic roadmap for facilities division based on scientific need
    - Who are our customers
    - What niche are facilities filling
    - What gaps should we fill

Implementation of Exascale Requirements Review (RR)

Series of workshops, one per SC Office (a hybrid between NERSC requirements reviews and Scientific Grand Challenges)

- **Location:** Washington DC area
- **Program Committee:** Representative community leaders from SC domain program office and ASCR facility staff
- **Attendance**: ~50 attendees including DOE program managers, DOE SC community representatives, ASCR supported applied mathematicians and computer scientists

Proposed Schedule

June 10-12,2015	HEP
November 3-5 2015	BES
January 27-29, 2016	FES
March 29-31, 2016	BER
June 15-17 2016	NP
Sept 27-29. 2016	ASCR

- **Agenda**: Plenary session and themed breakout sessions determined by program committee
- **Pre-meeting homework**: Templates will be developed and provided to chairs and attendees of breakout session for discussing and documenting data
  - White Papers: Broad coverage of Science area
  - Case Studies: Individual Examples
- **Output**: Summary workshop report written for each workshop.

Objectives of Current "Exascale" Requirements Review (RR)

Goal: Ensure the ability of ASCR facilities to support SC mission science in the exascale regime (2020-2025 timeframe).

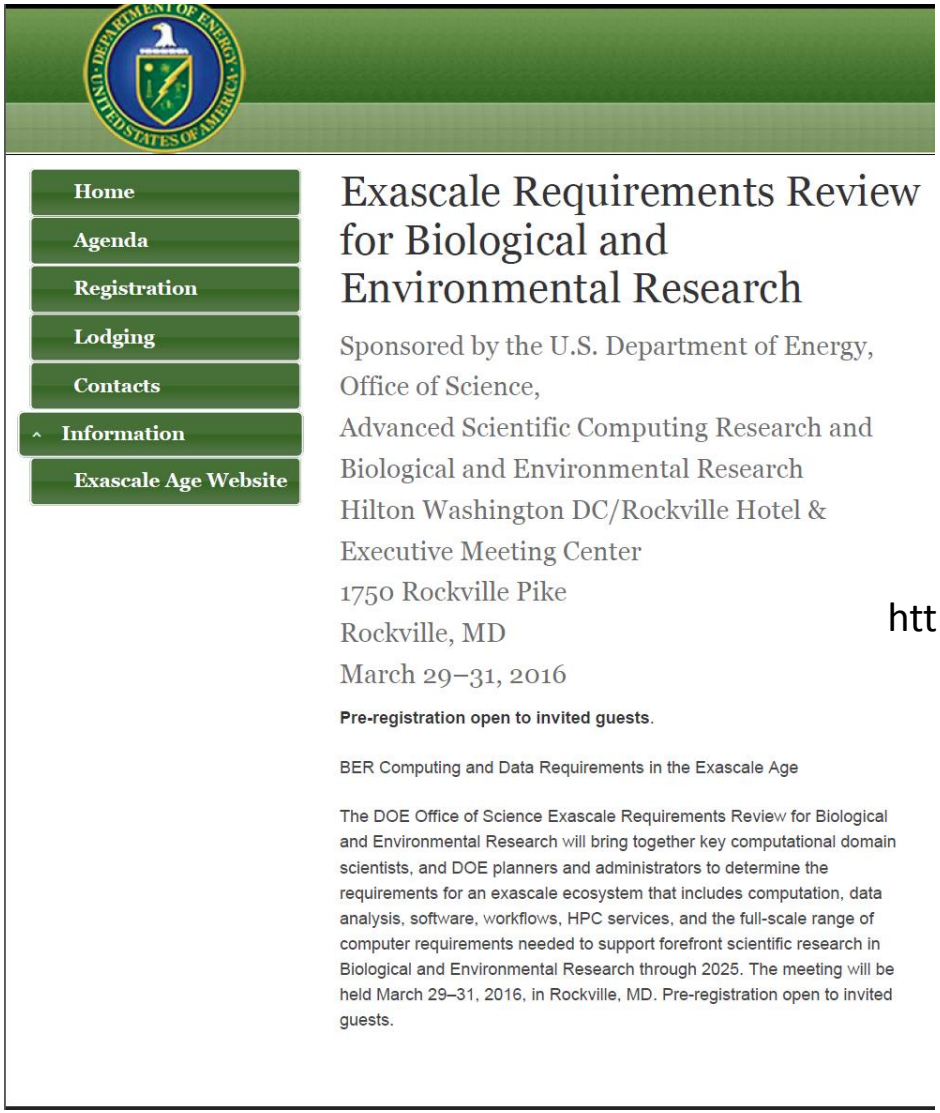
ASCR Research: Identify key computational science drivers that push exascale and describe **the HPC ecosystem** –HPC machine and related resources- needed to successfully accomplish your science goals

- Capture the whole picture:
  - Identify continuum of computing needs for the program office from institution clusters to Leadership computing.
    - » *Note: ASCR Facilities focus is on HPC and Leadership computing*.
  - Include modeling and simulation, scientific user facilities and large experiments needs, data needs, and near real time needs.
- Information gathered will inform the requirements for ecosystems for planned upgrades in 2020-2023 including the pre-exascale and exascale systems, network needs, data infrastructure, software tools and environments, and user services.

ASCR Facilities: Communicate to DOE SC scientists the known/fixed characteristics of upcoming compute system in the 2020-2025 timeframe and ask the computational scientists for feedback on proposed architectures.

Strengthen and inform interactions between HPC facility experts and scientists as well as ASCR Research and Facilities Divisions.

BER Exascale Requirements Review Workshop Web Page



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Exascale Age Website

Exascale Requirements Review for Biological and Environmental Research

Sponsored by the U.S. Department of Energy,
Office of Science,
Advanced Scientific Computing Research and
Biological and Environmental Research
Hilton Washington DC/Rockville Hotel &
Executive Meeting Center
1750 Rockville Pike
Rockville, MD
March 29–31, 2016

Pre-registration open to invited guests.

BER Computing and Data Requirements in the Exascale Age

The DOE Office of Science Exascale Requirements Review for Biological and Environmental Research will bring together key computational domain scientists, and DOE planners and administrators to determine the requirements for an exascale ecosystem that includes computation, data analysis, software, workflows, HPC services, and the full-scale range of computer requirements needed to support forefront scientific research in Biological and Environmental Research through 2025. The meeting will be held March 29–31, 2016, in Rockville, MD. Pre-registration open to invited guests.

https://www.orau.gov/berexascale2016/default.htm

ASCR-BER Requirements Workshop: March 29-30, 2016
Organizing committee and attendees

ASCR steering and organizing committees:

ORNL	Jack Wells, Tjerk Straatsma, James Hack
ANL	Paul Messina, Katherine Riley, Tim Williams, Richard Coffey
NERSC	Richard Gerber, Katie Antypas, Sudip Dosanjh
ASCR Program Office	Carolyn Lauzon

BER committee

CESD HQ POC: Dorothy Koch
Chair: Dave Bader
Breakout-Leads: Bill Collins, Ruby Leung and Mark Taylor, Minghua Zhang, Bill Gustafson, Peter Thornton, Dave Moulton, Todd Ringer, Wieslaw Maslowski, Phil Jones and Nathan Urban, Kate Calvin, Andy Jones, Esmond Ng, Kate Evans, Pat Worley, Rob Jacob, Dean Williams, Pavlos Kollias, Bert Debusschere, Hsi-Yen Ma, Gil Compo

BSSD HQ POC: Ramana Madupu
Chair: Adam Arkin
Breakout-Leads: Kathy Yelick, Eoin Brodie, Dan Rokhsar, Rich Bonneau, Lee Ann McCue, Tim Scheibe, Jeremy Smith, Matt Jacobson

ASCR-BER Requirements Workshop: March 29-30, 2016
Organizing committee and attendees

Community Attendees

- 41 BSSD (24 Lab, 17 University)
- 46 CESD (39 DOE-Lab; 7 University)

Attendees were encouraged to submit "Whitepaper Case-studies" for break-out discussion and for use in the report.

- 32 CESD 40 BSSD Whitepaper-case-studies were received before the meeting
- A few WP and CS were updated after the meeting to reflect discussions that occurred at the workshop

Status of Workshop Report

Report structure:

Executive Summary

1. Introduction

- **Goal of Exascale Reviews**
- **Workshop Structure and Report Preparation**

2. BER Vision and Mission

3. Research Directions and Computing Needs/Requirements

- **Breakout Topic 1**
  - **Scientific Challenges and Opportunities**
  - **Priority Research Directions**
  - **Cross-Cutting Research Directions**
  - **Computing Needs and Requirements**
- **Breakout Topic 2**
  - **Etc.**

4. Path Forward

Appendix (white papers and case studies)

Full draft expected January 2017