DOE Office of Advanced Scientific Computing Research

Presented to the

Advanced Scientific Computing Advisory Committee

by

Steve Binkley
Associate Director

September 20, 2016
Some Agenda Details

- **DATA FACILITY**
  - Kathy Yelick, Lawrence Berkeley National Laboratory

- **EXASCALE APPLICATIONS**
  - Doug Kothe, Oak Ridge National Laboratory

- **INTERNATIONAL HPC ACTIVITIES**
  - Jack Dongarra, UT and Oak Ridge National Laboratory

- **LABORATORY DIRECTED RESEARCH AND DEVELOPMENT (LDRD)**
  - John LaBarge, Director, Office of Lab Policy, Office of Science

- **FUTURE DIRECTIONS FOR NSF ADVANCED COMPUTING INFRASTRUCTURE**
  - Robert Harrison, Stony Brook University and Brookhaven National Laboratory

- **OFFICE OF SCIENCE EARLY CAREER RESEARCH PROGRAM**
  - Linda Blevins, Office of Science

- **OFFICE OF SCIENCE GRADUATE STUDENT RESEARCH PROGRAM**
  - James Glownia, Office of Science

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**Day 2**

- **EXPERIMENTAL AND OBSERVATIONAL DATA WORKSHOP FINDINGS AND RECOMMENDATIONS**
  - Wes Bethel, Lawrence Berkeley National Laboratory

- **THE ROLE OF HPC IN STOCKPILE STEWARDSHIP**
  - John L. Sarrao, Los Alamos National Laboratory

- **X-STACK PI MEETING UPDATE**
  - Vivek Sarkar, ASCAC and Rice University

- **THE ROLE OF HPC IN ADVANCED MANUFACTURING**
FY 2017 Budget

• Continuing Resolution for at least 3 months, possibly longer
• Impacts of House and Senate Energy & Water Development FY 2017 Marks
• Final resolution will await outcome of Presidential election
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<td><strong>5,347,000</strong></td>
<td><strong>5,672,069</strong></td>
<td><strong>+325,069 +6.1%</strong></td>
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</table>
Exascale – conduct research and development, and design efforts in hardware software, and mathematical technologies that will produce exascale systems for science applications

Facilities – acquire and operate more capable computing systems, from multi-petaflop through exascale computing systems that incorporate technologies emerging from research investments

Large Scientific Data – prepare today’s scientific and data-intensive computing applications to migrate to and take full advantage of emerging technologies from research, development and design efforts

Begin R&D for post-Moore Era
Continues support for the basic and applied research activities that support the broad scientific objectives of the Office of Science.

Activities on the critical path for the Exascale Computing Initiative (ECI) have been shifted to a new subprogram – the Exascale Computing Project (SC-ECP):

- ECI funds previously in other ASCR budget lines are aggregated into the SC-ECP subprogram
- Comprises R&D and delivery of exascale computers and will be managed following the principles of DOE Order 413.3B
- First four years focus on research in software (new algorithms and methods to support application and system software development) and hardware (node and system design), followed by acquisition of systems
- Project office established in FY 2016 at ORNL; Integrated Project Team across participating DOE/NNSA laboratories established in FY 2016

SciDAC (Scientific Discovery through Advanced Computing) partnerships will be re-competed in FY 2017.

Leadership Computing Facilities continue preparations for planned 75-200 petaflops upgrades at each site, to be completed in the 2018-2019 timeframe; National Energy Research Scientific Computing Center will begin operation of the NERSC-8 supercomputer (30 petaflops)

Modest effort in R&D for post-Moore’s Law computing included

Modest effort in support of BRAIN Initiative included, in collaboration with BER and BES

Computational Sciences Graduate Fellowship funded at $10 million
## ASCR – FY 2017 Funding Summary

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<td><strong>Mathematical, Computational, and Computer Sciences Research</strong></td>
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<td>(10,000)</td>
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<td>Computer Science</td>
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<td>55,259</td>
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<td>6,181</td>
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<td>High Performance Production Computing (NERSC)</td>
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<td>Leadership Computing Facilities</td>
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<td>Leadership Computing Facility at ANL (ALCF)</td>
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<td>81,796</td>
<td>77,000</td>
<td>77,000</td>
<td>80,000</td>
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<td>Leadership Computing Facility at ORNL (OLCF)</td>
<td>104,317</td>
<td>108,902</td>
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<td>Research and Evaluation Prototypes</td>
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<td>141,788</td>
<td>121,471</td>
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<td>(131,788)</td>
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<td>CSGF</td>
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<td>(10,000)</td>
<td>(10,000)</td>
<td>(...)</td>
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<td>...</td>
<td>...</td>
<td>154,000</td>
<td>+154,000 ...</td>
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<td>620,994</td>
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<td>663,180</td>
<td>+42,180 +6.8%</td>
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<td>------------------------------------------------------------</td>
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<td>Next Generation Networking for Science</td>
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<td>Total, Mathematical, Computational, and Computer Sciences Research</td>
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<td>179,176</td>
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<td>High Performance Production Computing (NERSC)</td>
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<td>Total, Leadership Computing Facilities</td>
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<td>181,317</td>
<td>181,317</td>
<td>187,000</td>
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<td>Research and Evaluation Prototypes</td>
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<td>(10,000)</td>
<td>(10,000)</td>
<td>(10,000)</td>
<td>(8,000)</td>
<td>(-20.0%)</td>
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<td>45,000</td>
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<td>441,824</td>
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<td>17-SC-20 Office of Science Exascale Computing Project (SC-ECP)</td>
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<td></td>
<td></td>
<td>154,000</td>
<td>-3,000</td>
<td>-1.9%</td>
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<td>621,000</td>
<td>621,000</td>
<td>663,180</td>
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<td>Computational Sciences Workforce Programs, with WDTs (non-add)</td>
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<td>(10,000)</td>
<td>(10,000)</td>
<td>(10,000)</td>
<td>(8,000)</td>
<td>(-20.0%)</td>
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<td>Exascale (non-add)</td>
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<td>(157,894)</td>
<td>(157,894)</td>
<td>(154,000)</td>
<td>(151,000)</td>
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<tr>
<td>Total, Exascale (non-add)</td>
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<td>621,000</td>
<td>621,000</td>
<td>663,180</td>
<td>663,180</td>
<td>621,000</td>
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Staffing Changes
Abani Patra

Program Manager in ASCR Applied Mathematics area

• EXPERIENCE
  – Professor, Department of Mechanical and Aerospace Engineering, University at Buffalo, State University of New York
  – Program Director Office of Cyberinfrastructure, National Science Foundation

• EDUCATION
  – University of Texas-Austin, Ph.D., Computational and Applied Mathematics
  – University of Missouri-Rolla, M.S., Mechanical Engineering
  – Birla Institute of Technology and Sciences, Pilani, India, B.E. Mechanical Engineering
Facilities Status
# ASCR Computing Upgrades At a Glance

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<th>System attributes</th>
<th>NERSC Now</th>
<th>OLCF Now</th>
<th>ALCF Now</th>
<th>NERSC Upgrade</th>
<th>OLCF Upgrade</th>
<th>ALCF Upgrades</th>
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<td>Name Planned Installation</td>
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<td>TITAN</td>
<td>MIRA</td>
<td>Cori 2016</td>
<td>Summit 2017-2018</td>
<td>Theta 2016</td>
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<td>System peak (PF)</td>
<td>2.6</td>
<td>27</td>
<td>10</td>
<td>&gt; 30</td>
<td>200</td>
<td>&gt;8.5</td>
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<td>Peak Power (MW)</td>
<td>2</td>
<td>9</td>
<td>4.8</td>
<td>&lt; 3.7</td>
<td>13.3</td>
<td>1.7</td>
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<td>Total system memory</td>
<td>357 TB</td>
<td>710TB</td>
<td>768TB</td>
<td>~1 PB DDR4 + HBM + 1.5PB persistent memory</td>
<td>&gt; 2.4 PB DDR4 + HBM + 3.7PB persistent memory</td>
<td>676 TB DDR4 + HBM</td>
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<td>Node performance (TF)</td>
<td>0.460</td>
<td>1.452</td>
<td>0.204</td>
<td>&gt; 3</td>
<td>&gt; 40</td>
<td>&gt; 3</td>
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<tr>
<td>Node processors</td>
<td>Intel Ivy Bridge</td>
<td>AMD Opteron Nvidia Kepler</td>
<td>64-bit PowerPC A2</td>
<td>Intel Knights Landing many core CPUs, Intel Haswell CPU in data partition</td>
<td>Multiple IBM Power9 CPUs &amp; multiple Nvidia Voltas GPUS</td>
<td>Intel Knights Landing Xeon Phi many core CPUs</td>
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<tr>
<td>System size (nodes)</td>
<td>5,600 nodes</td>
<td>18,688 nodes</td>
<td>49,152</td>
<td>9,300 nodes, 1,900 nodes in data partition</td>
<td>~4,600 nodes</td>
<td>&gt;3,200 nodes</td>
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<td>File System</td>
<td>7.6 PB 168 GB/s, Lustre®</td>
<td>32 PB 1 TB/s, Lustre®</td>
<td>26 PB 300 GB/s GPFS™</td>
<td>28 PB 744 GB/s Lustre®</td>
<td>120 PB 1 TB/s GPFS™</td>
<td>10PB, 210 GB/s Lustre initial</td>
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- Demand exceeds capability by 2×−6× across centers today
- Typical systems run at 80−90%+ utilization
Program Updates
Program Updates

• SciDAC-4:
  – Institutes extended through March 2017, leading to FOAs in FY 2017
  – Scope and approach for Partnerships under discussion with domain programs (BES, BER, FES, HEP, NP), leading to FOAs in FY 2017
    o Lessons learned, identification of new or additional partnership opportunities

• ASCR Long-Range Planning
  – Being led by Bill Harrod
  – Precursor to developing an ASCR strategic plan
  – In progress – will report on this during the December ASCAC meeting

• Moratorium on federal travel
  – In place through December 2016
  – Does not affect travel by national lab personnel or grantees
**Program Updates**

- **Exascale Computing Project (ECP)**
  - Critical Decision 0 (CD-0) approved by Deputy Secretary Sherwood-Randall on July 28, 2016
    - Guidance to develop option for earlier delivery of exascale systems
    - Direction to achieve CD-1/3A by November 2016
  - CD-1 review conducted Sept. 13-15, 2016
    - Some re-work necessary, mainly in documentation and life-cycle cost analysis
    - Major project features endorsed (approach, team, cost estimates)
  - Initial ECP applications selected (Doug Kothe’s presentation)
Previous Requirements Gathering Efforts: “Lead with the Science”

- 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
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 and a small number of Postdocs and senior CSGF fellows
- **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 case studies
- **Output:** Summary workshop report written for each workshop.

<table>
<thead>
<tr>
<th>Schedule</th>
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<tr>
<td>June 10-12, 2015</td>
<td>HEP</td>
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<tr>
<td>November 3-5, 2015</td>
<td>BES</td>
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<tr>
<td>January 27-29, 2016</td>
<td>FES</td>
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<td>March 29-31, 2016</td>
<td>BER</td>
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<tr>
<td>June 15-17, 2016</td>
<td>NP</td>
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<tr>
<td>Sept. 27-29, 2016</td>
<td>ASCR</td>
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</tbody>
</table>
• **Facilities needs**
  – Develop mission need statements for proposed upgrades (stretch your imaginations!!)
  – 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
Goal: Ensure the ability of ASCR facilities to support SC mission science in the exascale regime (2020-2025 timeframe).

Domain Program: Identify key computational science objectives that push exascale and describe the HPC ecosystem –HPC machine and related resources- needed to successfully accomplish the domain program’s science goals

• Capture the whole picture:
  – Identify continuum of computing needs for the program office from institution clusters to Leadership computing.
    » Note: ASCR 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: 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.
Requirements Reviews for ASCR Research
Gathering science drivers and requirements for the HPC ecosystem in 2020-2025

Website- http://www.orau.gov/ascrexascale2016/

- Rockville Hilton, September 27-28, 2016
- Headquarter’s POCs: Ceren Susut, Lucy Nowell, Betsy Riley, Carolyn Lauzon (ASCR)
- Conference Chairs: Jeffrey Vetter (ORNL), Ann Almgren (LBNL), Phil DeMar (FNAL)
- Registrants: 127 Registered Attendees (Lab, University, and a few industry Researchers, ASCR HPC and Networking Facility Staff, Laboratory Research Directors, ECP representatives, DOE program managers)

- **Agenda Contents**
  - Opening Talks (Barb Helland, Bill Harrod, ASCR)
  - Facility plans, resources, and activities, short summary of previous reviews (Katherine Riley, ANL)
  - ECP Update and Q&A (Paul Messina, ANL)
  - Breakout Sessions and Reporting throughout day 1 and 2
  - Day 3 - Begin writing

- **Breakout Sessions:**
  - Software Development
  - HPC Architectures
  - Distributed Computing and Networking (HPDC)
  - Data Management, Vis & Analytics
  - Systems Software Research
  - Production Systems: Operational Data & Policies
  - Production Systems: Software Deployment & Support

ASCAC September 20, 2016 20
Director, Office of Advanced Simulation and Computing and I R&D

NATIONAL NUCLEAR SECURITY ADMINISTRATION

Agency Contact Information

1 vacancy in the following location:

Washington DC, DC

Work Schedule is
PERMANENT/COMPETITIVE - PERMANENT

Opened Friday 9/16/2016
(3 day(s) ago)

Closes Thursday 10/6/2016
(17 day(s) away)

Salary Range
$161,903.00 to $185,100.00 / Per Year

Series & Grade
ES-0801, 1301-00/00

Promotion Potential
00

Supervisory Status
Yes

Who May Apply
Applications will be accepted from all United States citizens. You do not need to be a current or former federal employee to apply. Veterans preference does not apply to the SES.

Control Number
450675000

Job Announcement Number
NA-16-ES-012
Office of Advanced Scientific Computing Research

Associate Director – Steve Binkley
Phone: 301-903-7486
E-mail: Steve.Binkley@science.doe.gov

Research

Division Director – William Harrod
Phone: 301-903-5800
E-mail: William.Harrod@science.doe.gov

Facilities

Division Director – Barbara Helland
Phone: 301-903-9958
E-mail: Barbara.Helland@science.doe.gov

Relevant Websites
ASCRI:  science.energy.gov/ascr/
ASCRI Workshops and Conferences: science.energy.gov/ascr/news-and-resources/workshops-and-conferences/
ScIDAC: www.scidac.gov
INCITE:  science.energy.gov/ascr/facilities/incite/
Questions?
ASCAC LDRD Charge
Professor Daniel A. Reed, ASCAC Chair  
Office of the Vice President for Research and Economic Development  
University of Iowa  
2660 UCC  
Iowa City, IA 52242

May 19, 2016

Dear Professor Reed,

Thank you for your continued service to the Office of Science (SC) and the scientific communities that it serves as the Chair of the Advanced Scientific Computing Advisory Committee (ASCAC). Thank you for the committee’s latest report assessing the quality and effectiveness of the Office of Science and Technical Information’s (OSTI) recent and current products and services. This report will help both SC and OSTI transition its products and services to methods appropriate to the new era of information gathering and sharing.

I am writing to ask that ASCAC address a particularly important cross-cutting issue in the Department of Energy (DOE), namely an independent review of Laboratory Directed Research and Development (LDRD) work of the DOE Laboratories (Labs).

The objectives of the LDRD program are to: (1) maintain the scientific and technical vitality of the Labs; (2) enhance the Labs’ ability to address current and future DOE and National Nuclear Security Administration (NNSA) missions; (3) foster creativity and stimulate exploration of forefront science and technology; (4) serve as a proving ground for new concepts in R&D; and (5) support high-risk, potentially high-value R&D. DOE policy allows the Secretary of Energy to authorize up to 6% of a DOE Lab’s total operating and capital equipment budget, including non-DOE funded work, for LDRD work.

The June 17, 2015, interim report of the Secretary of Energy Advisory Board (SEAB) Task Force on DOE National Laboratories recommended an independent peer review of the LDRD program impacts and process of four laboratories, evaluating up to ten years of funded projects. I am asking ASCAC to review the LDRD program processes and the impact of LDRD at four of the DOE Labs, to include at least one SC Lab, one NNSA Lab, and one of the applied energy Labs. Please choose Labs that have had LDRD programs for at least ten years.

In your review, please consider each Lab’s processes to:
- determine the funding levels for the LDRD programs;
- determine Lab-specific goals and allocate resources among the goals;
- select specific projects; and
- evaluate the success and impact of the LDRD program against Lab-specific goals and the overall objectives of the LDRD program over a ten-year period.

In assembling a subcommittee, please consider members of or recommendations from the other Office of Science Federal advisory committees, the Defense Programs Advisory Committee, the Environmental Management Advisory Board, and the Nuclear Energy Advisory Committee.

The output of this review should be a brief report with an Executive Summary suitable for a general audience. The report should be available in the spring of 2017. We look forward to the results of your review and any recommendations that result from this study.

Sincerely,

C. A. Murray  
Director, Office of Science
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