

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

Day 1

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

Day 2

- 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
 - Mark Johnson, U.S. Department of Energy Office of Energy Efficiency and Renewable Energy



FY 2017 Budget

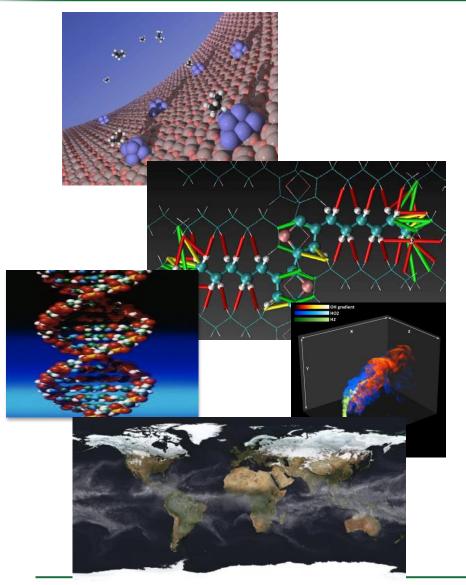
- Continuing Resolution for at least 3 months, possibly longer
- Impacts of House and Senate Energy & Water Development FY 2017 Marks
- Final resolution will await outcome of Presidential election

Office of Science FY 2017 Budget Request to Congress (Dollars in thousands)

	FY 2015 Enacted Approp.	FY 2015 Current Approp.	FY 2016 Enacted Approp.	FY 2017 President's Request	FY 2017 Presi vs. FY 2016 Appro	Enacted
Science						
Advanced Scientific Computing Research	541,000	523,411	621,000	663,180	+42,180	+6.8%
Basic Energy Sciences	1,733,200	1,682,924	1,849,000	1,936,730	+87,730	+4.7%
Biological and Environmental Research	592,000	572,618	609,000	661,920	+52,920	+8.7%
Fusion Energy Sciences	467,500	457,366	438,000	398,178	-39,822	-9.1%
High Energy Physics	766,000	745,232	795,000	817,997	+22,997	+2.9%
Nuclear Physics	595,500	580,744	617,100	635,658	+18,558	+3.0%
Workforce Development for Teachers and Scientists	19,500	19,500	19,500	20,925	+1,425	+7.3%
Science Laboratories Infrastructure	79,600	79,600	113,600	130,000	+16,400	+14.4%
Safeguards and Security	93,000	93,000	103,000	103,000		
Program Direction	183,700	183,700	185,000	204,481	+19,481	+10.5%
University Grants (Mandatory)				100,000	+100,000	
Small Business Innovation/Technology Transfer Research (SC)		132,905				
Subtotal, Science	5,071,000	5,071,000	5,350,200	5,672,069	+321,869	+6.0%
Small Business Innovation/Technology Transfer Research (DOE)		65,075				
Rescission of Prior Year Balance	-3,262	-3,262	-3,200		+3,200	-100.0%
Total, Science	5,067,738	5,132,813	5,347,000	5,672,069	+325,069	+6.1%



ASCR Investment Priorities



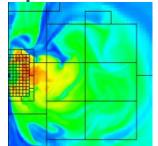
- Exascale conduct research and development, and design efforts in hardware software, and mathematical technologies that will produce exascale systems for science applications
- Facilities acquire and operate more capable computing systems, from multipetaflop through exascale computing systems that incorporate 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

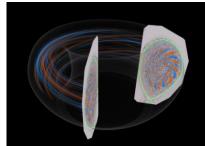


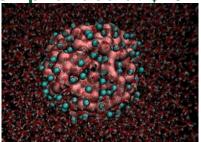
ASCR FY 2017 Budget Highlights

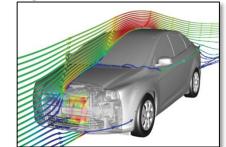
- Continues support for the basic and applied research activities that support the broad scientific objectives of the Office of Science
- Activities on the critical path for the Exascale Computing Initiative (ECI) have been shifted to a new subprogram – the Exascale Computing Project (SC-ECP):
 - ECI 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 recompeted 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









ASCAC September 20, 2016

ASCR – FY 2017 Funding Summary

					1		
	FY 2015	FY 2015	FY 2016	FY 2016	FY 2017	FY 2017 P	
	Enacted	Current	President's	Enacted	President's	Req. vs. I	
	Approp.	Approp.	Request	Approp.	Request	Enacted .	Approp.
Mathematical, Computational, and Computer Sciences Research							
Applied Mathematics	49,155	49,454	49,229	49,229	*	-10,000	-20.3%
Exascale	(5,000)	(5,000)	(5,000)	(10,000)	()	(-10,000)	(-100.0%)
Computer Science	55,767	55,259	•	56,848		-17,552	-30.9%
Exascale	(20,000)	(20,000)	(25, 106)	(20,423)	()	(-20, <i>4</i> 23)	(-100.0%)
Computational Partnerships (SciDAC)	46,918	43,996	47,918	47,918	45,596	-2,322	-4.8%
Exascale	(16,000)	(16,000)	(16,000)	(16,000)	()	(-16,000)	(-100.0%)
Next Generation Networking for Science	19,000	19,011	19,000	19,000	19,000		
SBIR/STTR	5,830		6,181	6,181	7,733	+1,552	+25.1%
Total, Mathematical, Computational, and Computer Sciences							
Research	176,670	167,720	179,170	179,176	150,854	-28,322	-15.8%
High Performance Computing and Network Facilities							
High Performance Production Computing (NERSC)	75,605	75,905	76,000	86,000	92,145	+6,145	+7.1%
Leadership Computing Facilities							
Leadership Computing Facility at ANL (ALCF)	80,320	81,796	77,000	77,000	80,000	+3,000	+3.9%
Leadership Computing Facility at ORNL (OLCF)	104,317	108,902	94,000	104,317	107,000	+2,683	+2.6%
Total, Leadership Computing Facilities	184,637	190,698	171,000	181,317	187,000	+5,683	+3.1%
Research and Evaluation Prototypes	57,329	53,298	141,788	121,471	17,890	-103,581	-85.3%
Exascale	(50,000)	(50,000)	(131,788)	(111,471)	()	(-111,471)	(-100.0%)
CSGF	(3,000)	(3,000)	(10,000)	(10,000)	(10,000)	()	()
High Performance Network Facilities and Testbeds (ESnet)	35,000	35,790	38,000	38,000	45,000	+7,000	+18.4%
SBIR/STTR	11,759		15,036	15,036	16,291	+1,255	+8.3%
Total, High Performance Computing and Network Facilities	364,330	355,691	441,824	441,824	358,326	-83,498	-18.9%
Exascale Computing							
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)					154,000	+154,000	
Total, Advanced Scientific Computing Research	541,000	523,411	620,994	621,000	663,180	+42,180	+6.8%



	FY 2016 President' s Request			FY 2017 President's Request	FY 2017 House Mark	FY 2017 House vs. FY 2017 Request		FY 2017 FY 2017 Senate vs. FY 2017 Mark Request		017
Mathematical, Computational, and Computer Sciences Research										
Applied Mathematics	49,229	49,229	49,229	39,229	29,229	-10,000	-25.5%	37,229	-2,000	-5.1%
Exascale	(5,000)	(10,000)	(10,000)	()	()	()	()	()	()	()
Computer Science	56,842	56,848	56,848	39,296	29,296	-10,000	-25.4%	37,296	-2,000	-5.1%
Exascale	(25,106)		(20,423)	()	()	()	()	()	()	()
Computational Partnerships (SciDAC)	47,918	47,918	47,918	45,596	32,596	-13,000	-28.5%	40,596	-5 000	-11.0%
Exascale	(16,000)		-	()	()	()	()	()	()	()
Next Generation Networking for Science	19,000		19,000		16,000	` '	-15.8%	18,255	-745	-3.9%
SBIR/STTR	6,181	6,181	6,181	7,733	6,369		-17.6%	7,364	-369	-4.8%
Total, Mathematical, Computational, and Computer										
Sciences Research	179,170	179,176	179,176	150,854	113,490	-37,364	-24.8%	140,740	-10,114	-6.7%
High Performance Computing and Network Facilities										
High Performance Production Computing (NERSC)	76,000	86,000	86,000	92,145	92,145			92,145		
Leadership Computing Facilities										
Leadership Computing Facility at ANL (ALCF)	77,000	77,000	77,000	80,000	80,000			80,000		
Leadership Computing Facility at ORNL (OLCF)	94,000	,	-	107,000	110,000		+2.8%	110,000	+3,000	
Total, Leadership Computing Facilities	171,000	181,317	181,317	187,000	190,000	+3,000	+1.6%	190,000	+3,000	+1.6%
Research and Evaluation Prototypes	141,788	121,471	121,471	17,890	13,250	-4,640	-25.9%	17,890		
Exascale	(131,788)	(111,471)	(111,471)	()	()	()	()	()	()	()
CSGF	(10,000)	(10,000)	(10,000)	(10,000)	(8,000)	(-2,000)	(-20.0%)	(10,000)	()	()
High Performance Network Facilities and Testbeds										
(ESnet)	38,000	38,000	38,000	45,000	45,000			45,000		
SBIR/STTR	15,036	15,036	15,036	16,291	16,115	-176	-1.1%	16,405	+114	+0.7%
Total, High Performance Computing and Network										
Facilities	441,824	441,824	441,824	358,326	356,510	-1,816	-0.5%	361,440	+3,114	+0.9%
Exascale Computing										
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)				154,000	151,000	-3,000	-1.9%	154,000		
Total, Advanced Scientific Computing Research	620,994	621,000			621,000		-6.4%	656,180	-7,000	-1.1%
Computational Sciences Workforce Programs, with										
WDTS (non-add)		(10,000)		(10,000)	(8,000)	(-2,000)		(10,000)	()	()
Exascale (non-add)		(157,894)					(-1.9%)	(154,000)	()	(8
	620,994	621,000	621,000	663,180	621,000			656,180	J	

Staffing Changes

ASCR Staffing – New Program Manager

Applied Mathematics

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

System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	NERSC Upgrade OLCF Upgrade		CF Upgrades
Name Planned Installation	Edison	TITAN	MIRA	Cori 2016	Summit 2017-2018	Theta 2016	Aurora 2018-2019
System peak (PF)	2.6	27	10	> 30	200	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	13.3	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + HBM+1.5PB persistent memory	> 2.4 PB DDR4 + HBM + 3.7 PB persistent memory	676 TB DDR4 + HBM	> 7 PB HBM, Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~4,600 nodes	>3,200 nodes	>50,000 nodes
File System	7.6 PB 168 GB/s, Lustre [®]	32 PB 1 TB/s, Lustre [®]	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre [®]	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre [®]

- 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
 - 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"









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



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 and a small number of Postdocs and senior CSGF fellows

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 case studies
- Output: Summary workshop report written for each workshop.



Requirements Reviews Need to Meet Multiple Needs

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



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).

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/

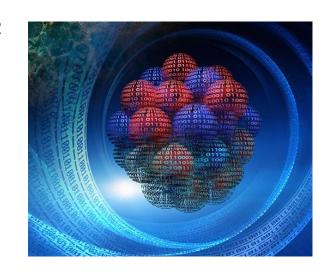
- Rockville Hilton, September 27-28, 2016
- Headquarter's POCs: Ceren Susut, Lucy Nowell, Betsy Riley, Carolyn Lauzon (ASCR)
- Conference Chairs: Jeffrey Vetter (ORNL), Ann Almgren (LBNL), Phil DeMar (FNAL)
- Registrants: 127 Registered Attendees (Lab, University, and a few industry Researchers, ASCR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

Agenda Contents

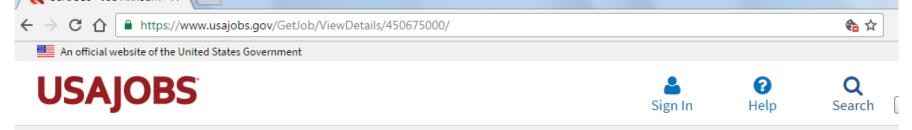
- Opening Talks (Barb Helland, Bill Harrod, ASCR)
- Facility plans, resources, and activities, short summary of previous reviews (Katherine Riley, ANL)
- ECP Update and Q&A (Paul Messina, ANL)
- Breakout Sessions and Reporting throughout day 1 and 2
- Day 3 Begin writing

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







Create an account to get started — build your profile, create or upload resumes and apply for jobs.

https://www.usajobs.gov/GetJob/ViewDetails/450675000/

Director, Office of Advanced Simulation and Computing and I R&D

NATIONAL NUCLEAR SECURITY ADMINISTRATION

Agency Contact Information

1 vacancy in the following location: Salary Range \$161,903.00 to \$185,100.00 / Per Year Washington DC, DC Series & Grade Work Schedule is PERMANENT/COMPETITIVE - PERMANENT ES-0801, 1301-00/00 Promotion Potential Opened Friday 9/16/2016 (3 day(s) ago) 00 O Closes Thursday 10/6/2016

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



(17 day(s) away)





Apply

ASCR at a Glance

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

ASCR: <u>science.energy.gov/ascr/</u>

ASCR 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

ASCAC Charge to Review DOE LDRD Program

May 19, 2016



Office of Science Washington, DC 20585

May 19, 2016

Office of the Direct

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

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, the 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

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Director, Office of Science

ASCAC Charge to Review DOE LDRD Program May 19, 2016

The June 17, 2015, the 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.

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