U.S. DEPARTMENT OF ENERGY

DOE Office of Advanced Scientific Computing Research

Presented to the

Advanced Scientific Computing Advisory Committee

by

Barbara Helland
Acting Associate Director

December 20, 2016

Some Agenda Details

- **UPDATE ON THE EXASCALE COMPUTING PROJECT**
  - *Paul Messina, ECP Director*
- **THE NEED FOR A NEW PUBLIC-PRIVATE PARTNERSHIP IN MICROELECTRONICS**
  - *Deborah Wince-Smith, Council on Competitiveness*
- **ASCR'S PRELIMINARY PLAN FOR COMPUTING "BEYOND MOORE'S LAW"**
  - *Ceren Susut-Bennett, ASCR*
- **FPGAS FOR SUPERCOMPUTING: THE WHY AND HOW**
  - *Hal Finkel, Argonne National Laboratory*
- **LONG RANGE PLANNING ACTIVITY**
  - *Bill Harrod, ASCR*
- **UPDATE ON LDRD SUBCOMMITTEE**
  - *Martin Berzins, ASCAC*
- **TOOL FOR ESTIMATING RETURN ON INVESTMENTS FROM HPC**
  - *Earl Joseph, IDC*

Staffing Changes

SC Transition Leadership

- **Office of the Director** — ***Cherry Murray***
  - **Deputy Director for Field Operations** — *Joseph McBrearty*; Associate Deputy – *Stephanie Short*
    - Ames Site Office — *Cynthia Baebler*
    - Argonne Site Office — *Joanna Livengood*
    - Berkeley Site Office — *Paul Golan*
    - Brookhaven Site Office — *Frank Crescenzo*
    - Fermi Site Office — *Michael Weis*
    - Thomas Jefferson Site Office — *Joseph Arango*
    - ORNL Site Office — *Johnny Moore*
    - Princeton Site Office — *Peter Johnson*
    - Pacific NW Site Office — *Roger Snyder*
    - SLAC Site Office — *Paul Golan*
    - Chicago Office — *Roxanne Purucker*
    - SC Integrated Support Center
    - Oak Ridge Office — *Kenneth Tarcza*
    - Office of Safety and Security Policy — *Todd Lapointe*
    - Office of Laboratory Policy — *John LaBarge*
    - Office of Operations Program Management — *C. Steve Trischman*
  - **Deputy Director for Science Programs** — *J. Steven Binkley*
    - Advanced Scientific Computing Research — *Barbara Helland (acting)*
    - Basic Energy Sciences — *Harriet Kung*
    - Biological & Environmental Research — *Sharlene Weatherwax*
    - Fusion Energy Sciences — *Edmund Synakowski*
    - High Energy Physics — *James Siegrist*
    - Nuclear Physics — *Timothy Hallman*
    - Workforce Development f/Teachers & Scientists — *James Glownia*
    - Project Assessment — *Stephen Meador*
    - SBIR/STTR Programs Office — *Manuel Oliver*
  - **Deputy Director for Resource Management** — *Jeffrey Salmon*; Executive Officer - *Helen DeHart*
    - Budget — *Kathleen Klausing*
    - Grants & Contracts — *Michael Zarkin (A)*
    - Scientific and Technical Information — *Brian Hitson*
    - Information Technology and Services — *Vasilios Kountouris*
    - SC Communications and Public Affairs — *Rick Borchelt*
    - Office of Management — *Cynthia Mays*

Slides presented at an SC All Hand's Meeting October 5, 2017 by Dr. Murray

Associate Director of
Advanced Scientific Computing Research

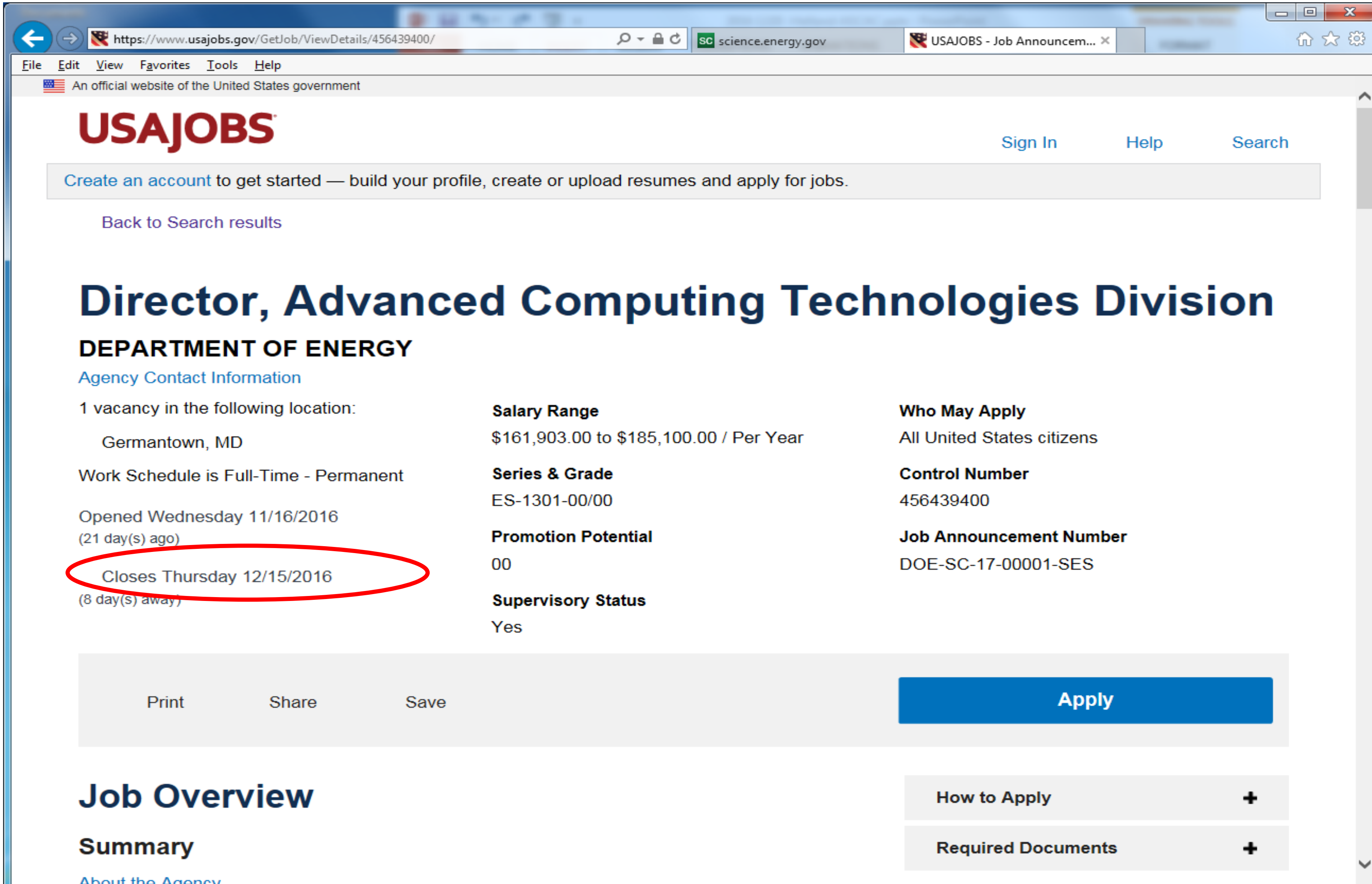
Barbara Helland, Associate Director (Acting)

Computational Science and Partnerships (SciDAC) Division
William Harrod, Director

Facilities Division
Christine Chalk, Director (Acting)

Advanced Computing Technologies Division
Director - Vacant

Division Director Job Posting



https://www.usajobs.gov/GetJob/ViewDetails/456439400/ | science.energy.gov | USAJOBS - Job Announcem...

File Edit View Favorites Tools Help

An official website of the United States government

USAJOBS

Sign In Help Search

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

Back to Search results

Director, Advanced Computing Technologies Division

DEPARTMENT OF ENERGY

Agency Contact Information

1 vacancy in the following location:

Germantown, MD

Work Schedule is Full-Time - Permanent

Opened Wednesday 11/16/2016
(21 day(s) ago)

Closes Thursday 12/15/2016
(8 day(s) away)

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

Series & Grade
ES-1301-00/00

Promotion Potential
00

Supervisory Status
Yes

Who May Apply
All United States citizens

Control Number
456439400

Job Announcement Number
DOE-SC-17-00001-SES

Print Share Save

Apply

Job Overview

Summary

About the Agency

How to Apply +

Required Documents +

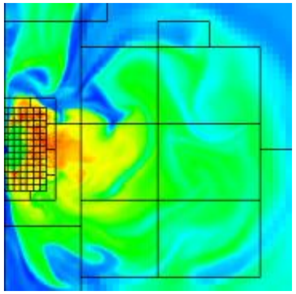
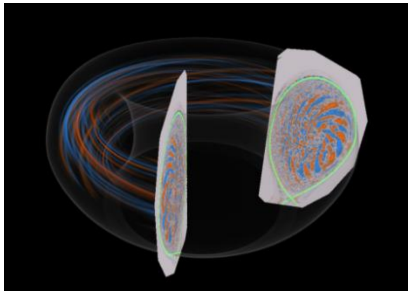
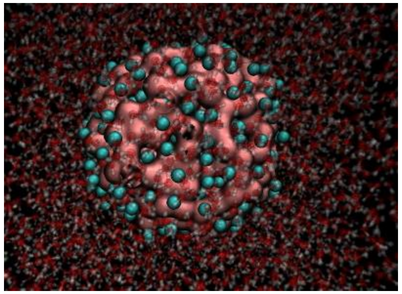
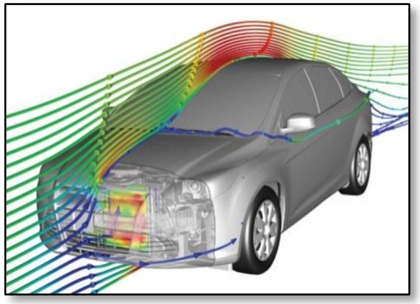
FY 2017 Budget

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
  - 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 PF 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 PF)**
- **Computational Sciences Graduate Fellowship funded at $10 million**

New Starts

- ***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***

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 President's Req. vs. FY 2016 Enacted Approp.	
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%**

Continuing Resolutions

- **H.R.5325 - Continuing Appropriations and Military Construction, Veterans Affairs, and Related Agencies Appropriations Act, 2017, and Zika Response and Preparedness Act**
  - Such amounts as may be necessary, at a rate for operations as provided in the applicable appropriations Acts for fiscal year 2016
  - The rate for operations provided by subsection (a) is hereby reduced by 0.496 percent.
- **H.R. 2028 The Senate Amendment To H.R. 2028, Energy and Water Development and Related Agencies Appropriations Act, 2016**
  - Amended previous CR bill to change the date to April 28, 2017 and
  - Lower the reduction from 0.496 percent to 0.1901 percent

ASCR 2017 Budget Overview

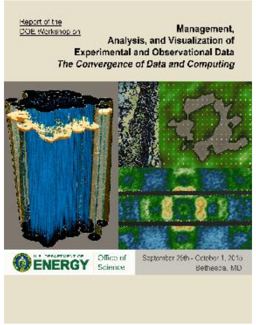
	FY 2015 Approp.	FY 2016 Approp.	FY 2017 President's Request	*FY 2017 House Mark*	*FY 20167 Senate Mark*
Advanced Scientific Computing Research					
Applied Mathematics	49,155	49,229	39,229	29,229	37,229
Exascale	*(5,000)*	*(10,000)*			
Computer Science	55,767	56,848	39,296	29,296	37,296
Exascale	*(20,000)*	*(20,423)*			
Computational Partnerships (SciDAC)	46,918	47,918	45,596	32,596	40,596
Exascale	*(16,000)*	*(16,000)*			
Next Generation Networking for Science	19,000	19,000	19,000	16,000	18,255
SBIR/STTR	5,830	6,181	7,733	6,369	7,364
Total, Mathematical, Computational, and Computer Sciences Research	***176,670***	***179,176***	***150,854***	**113,490**	***140,740***
High Performance Production Computing (NERSC)	75,605	86,000	92,145	92,145	92,145
Leadership Computing Facilities	184,637	181,317	187,000	190,000	190,000
Research and Evaluation Prototypes	57,329	121,471	17,890	13,250	17,890
Exascale	*(50,000)*	*(111,471)*			
CSGF	*(3,000)*	*(10,000)*	*(10,000)*	*(8,000)*	*(10,000)*
High Performance Network Facilities & Testbeds (ESnet)	35,000	38,000	45,000	45,000	45,000
SBIR/STTR	11,759	15,036	16,291	16,115	16,405
Total, High Performance Computing and Network Facilities	***364,330***	***441,824***	***358,326***	***356,510***	***361,440***
SC – Exascale Computing Project			154,000	151,000	154,000
Total, Advanced Scientific Computing Research	**541,000**	**621,000**	**663,180**	**621,000**	**656,180**

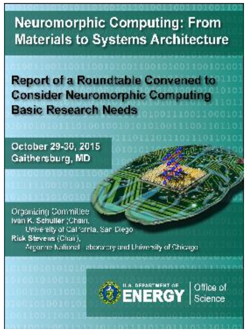
U.S. DEPARTMENT OF ENERGY

Research Updates

ASCR's Research

- **Applied Mathematics**
  - *Supports the research and development of applied mathematics models, methods and algorithms for understanding natural and engineered systems related to DOE's mission with a focus on discovery of new applied mathematics, for the ultra-low power, multicore-computing, and data-intensive future;*
- **Computer Science**
  - *Supports the research and development of today's and tomorrow's leading edge computers tools for DOE science and engineering and extracting scientific information, discovery and insight from massive data from experiments and simulations;*
- **Partnerships**
  - *CoDesign and SciDAC partnerships to pioneer the future of scientific applications;*
- **Next Generation Networks for Science**
  - *Building upon results from Computer Science and Applied Mathematics, supports research and development of integrated software tools and advanced network services to use new capabilities in ESnet to integrate science workflows to network infrastructures and experiments and enable large-scale scientific collaborations.*





FY16 ASCR Early Career Awardees

	PI	Institution	Title	Topic Area
	**Travis Humble PhD: 2005**	Oak Ridge National Laboratory	Accelerating Applications of High-Performance Computing with Quantum Processing Units	Beyond CMOS
	**Clayton Webster PhD: 2007**	Oak Ridge National Laboratory	Mathematical Methods for Optimal Polynomial Recovery of High-Dimensional Systems from Noisy Data	Applied Math
	**Yier Jin PhD: 2012**	University of Central Florida, Orlando, FL	Resilient and Robust High Performance Computing Platforms for Scientific Computing Integrity	Cybersecurity
	**Alvin Cheung PhD: 2015**	University of Washington, Seattle, WA	Using Verified Lifting to Optimize Legacy Stencil Codes	Software Stack

FY16 ASCR National Laboratory Winners

Travis Humble – Oak Ridge National Laboratory; Beyond CMOS

PhD: 2005 PhD in Theoretical Chemistry, University of Oregon

Title: Accelerating Applications of High-Performance Computing with Quantum Processing Units

Overview: This is an exploratory research to study the performance of quantum-enabled HPC systems running scientific computing applications. Specifically the role of Quantum Processing Units (QPUs) will be studied in depth. The uniqueness of this study is in the overall system-level simulation of quantum-enabled HPC applications.

Clayton Webster – Oak Ridge National Laboratory; Applied Math

PhD: 2007 PHD in Applied Mathematics, Florida State University

Title: Mathematical Methods for Optimal Polynomial Recovery of High-Dimensional Systems from Noisy Data

Overview: The proposed research is at the forefront of approximation theory, uncertainty quantification, and scalable algorithms for the analysis and reconstruction of solutions from high-dimensional, parameterized, computational models. For complex problems, accuracy and efficiency are important criteria in constructing high-dimensional solution maps from expensive numerical simulations or noisy data from time-consuming physical experiments. The research includes new ways to compute accurate, short-term expansions of functions, and a variety of approaches for constructing reduced-order models. The research will also be applied to parameterized problems in optimal control, where the function approximation techniques can be used to enhance the efficiency for optimization.

FY16 ASCR University Winners

Yier Jin – University of Central Florida; Cybersecurity
PhD: 2012 PhD in Electrical Engineering, Yale University
Title: Resilient and Robust HPC Platforms for Scientific Computing Integrity
Overview: Heterogeneous HPC platform with intrusion detection, access control, and memory protection that is scalable to the protection required, transparent to user/administrator, adaptable to the security arms-race, and highly efficient. It leverages micro-architectural and OS features to dynamically protect applications. The proposed hardware-assisted solution will help reshape current and future HPC platforms such that platform security and data integrity become intrinsic to HPC deployment.

Alvin Cheung – University of Washington; Software Stack
PhD: 2015 PhD in Computer Science, Massachusetts Inst. of Technology
Title: Using Verified Lifting to Optimize Legacy Stencil Codes
Overview: The proposed methods enable verifiable transformations of low level implementations into mathematical intermediate representations, which are formally proven correct and then transformed to efficient implementations on a variety of platforms. The proposed approach eliminates the need for manual rewrites or the need for devising translation rules to compile the source to the target Domain Specific Language (DSL), which are time consuming and error-prone. The proposed methods ensure the correctness of the automated transformations.

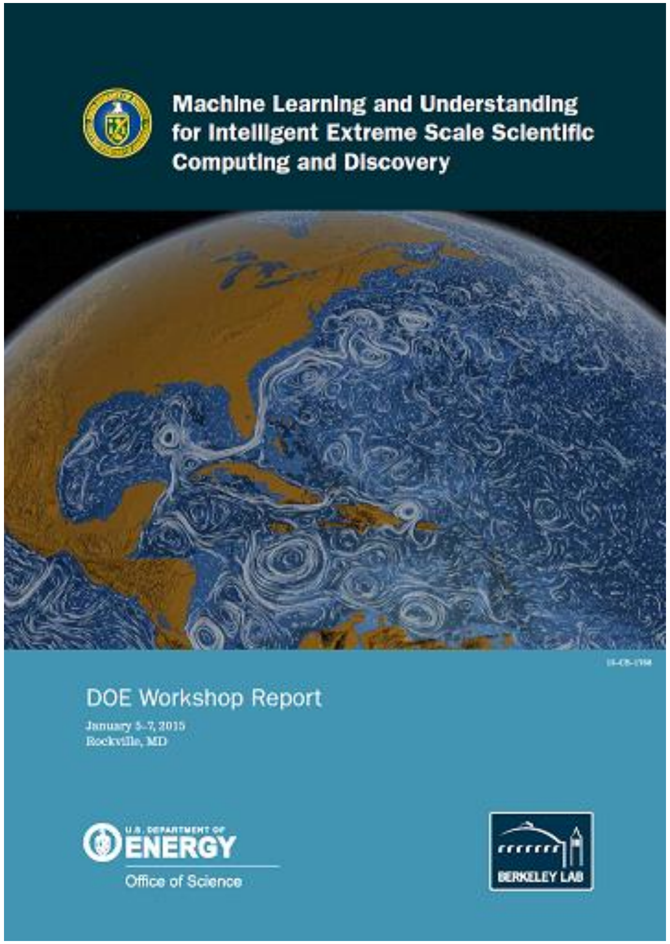
Early Career

- **Proposals for the 8th cohort of Early Career awardees were due on November 14, 2016 and are currently under review.**
- **ASCR's anticipates selecting 4 University and 3 Laboratory Early Career awardees in 2017.**

The National Artificial Intelligence Research And Development Strategic Plan

- **In 2015, DOE ASCR sponsored an Artificial Intelligence workshop:**
  - The 2015 Machine Learning and Understanding For Scientific Discovery Workshop
    - The workshop focused on three technological areas: Self-aware runtime and operating systems, Deep learning for big data, and Resiliency and Trust.

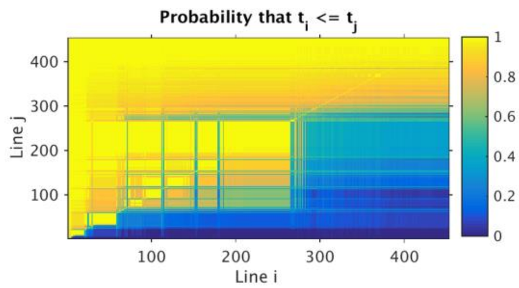
- **In 2016, these AI activities led DOE to release a Funding Opportunity Announcement titled "Machine Learning and Understanding for High Performance Computing Scientific Discovery"**
  - In this topic area, research proposals may cover supervised, unsupervised, reinforced learning, or variants such as semi supervised learning for example.
    - ASCR is currently in the award process



Mathematical Multifaceted Integrated Capability Centers (MMICCs)

Goal:

Address long-term mathematics research challenges with impact to the DOE mission *in the 5-10+ year timeframe.*

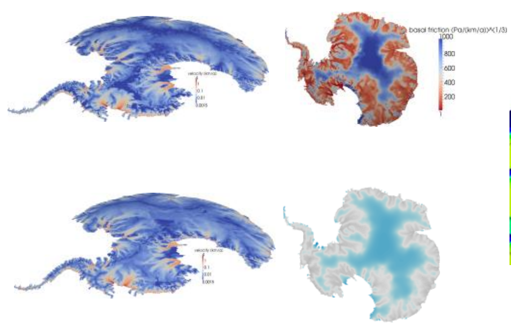


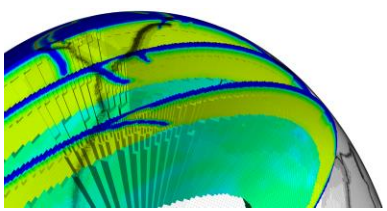
Outcomes/Performance Measures:

~(86+95+148)=~329 publications in peer reviewed literature in 4 years!

Greater than 30 faculty and lab researchers trained.

Gordon Bell, SIAM fellows,…





MMICCS have been very successful and can serve to anchor DOE Office of Science investments in Applied Math.

Long-Term DOE Impact:

New mathematics at the intersection of multiple mathematical sub-domains – data driven discovery, multi-scale modeling, grid optimization, large scale inversion, rare events …

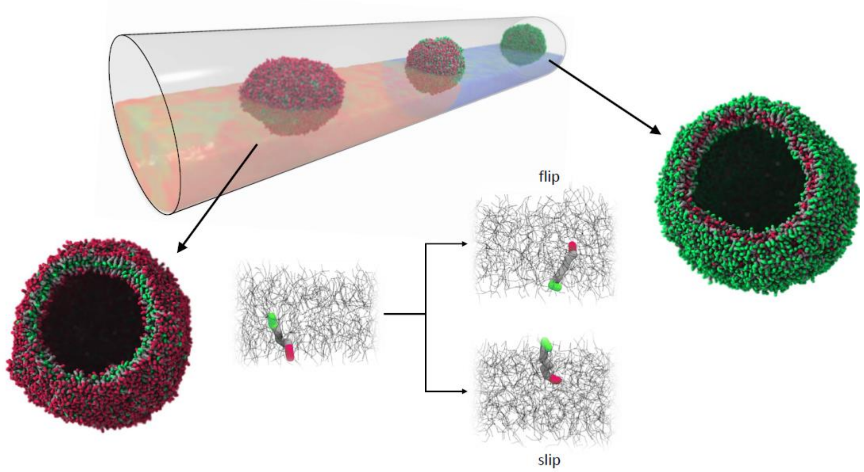
- Several high impact "application transitions" – Grid Modernization Laboratory Consortium (GMLC), Exascale Application Project, partnerships with Center for Integrated Nanotechnologies, Material Synthesis and Simulation Across Scales …
- DOE's Quadrennial technology review (QTR) feature.

Mathematical Multifaceted Integrated Capability Centers (MMICCs)

Program Review:

Program went through careful review process in Oct-Nov 16.

- 1.5 day reverse site visit format with detailed report prior to review and written Q&A
- 1 day study group with selected researchers, PIs and other agency program managers on best practices and lessons learnt in such focused investments for Applied Mathematics



Outcomes:

Reviews and study group were very positive on the program and in addition to the many research highlights, notes on best practices and kudos, suggestions for improvement commented thus:

“The collective group of people involved in this round of MMICCs **would never had embarked on this successful line of research without the MMICCs program**."

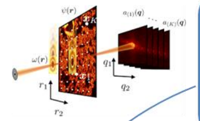
Long-Term DOE Impact:

Core groups of organized researchers from multiple laboratories and leading university groups with great intellectual ability, diverse skills and experience levels have assembled to successfully, tackle grand challenge problems.

Challenge is to sustain and adapt groups to evolving needs in mission related research.

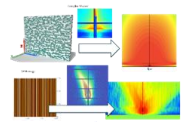
The Center for Advanced Mathematics for Energy Research Applications

Building the mathematics that transforms data into information.



Real-time streaming ptychography—ALS, delivered to NSLS2, LANL, BESSY,

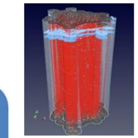
Designing mathematical algorithms to allow real-time analysis next to the equipment



SFM/TEM + GISAXS

Multi-modal: Building the math that fuses information from multiple experiments

New algorithms to transform manual into automatic analysis

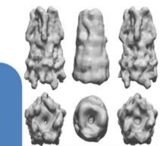


Automatic image processing for the ALS/GE

CAMERA workshop on Tomography: Joint with APS, ESRF, DIAMOND, LNLS, LLNL, SSRL,....,

Compare and integrate multiple analysis tools

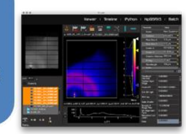
Inventing new math and models to match new acquisition technologies



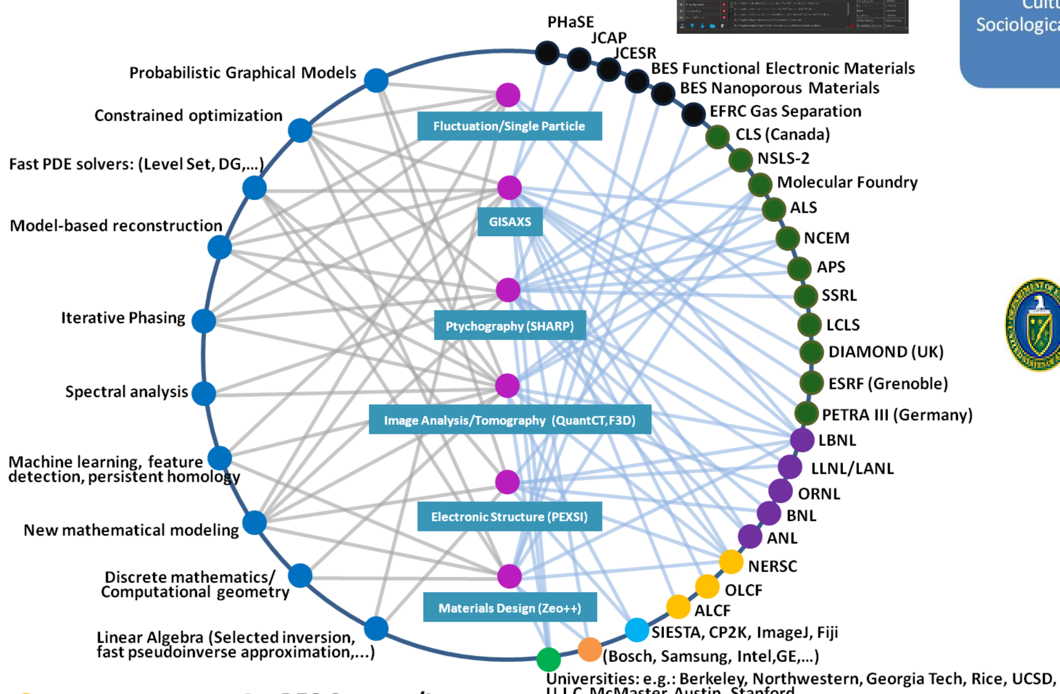
Fluctuation scattering and single particle imaging for the LCLS

Cultural and Sociological Challenges

Robust and reliable codes and data flow: workflow environments



Workflow and access to remote supercomputers: XiCAM for ALS, SSRL, APS, NSLS2



=ASCR Facilities =BES Centers/Internat.
=BES (and other) Facilities =LABS =3Rd Party Codes =Universities

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

ALS ADVANCED LIGHT SOURCE

Advanced Photon Source Argonne National Laboratory

LCLS

SSRL

MOLECULAR FOUNDRY

Smart Networks
(Towards Autonomic Cyber-Facilities)

December 8-9, 2016, Hilton Hotel, Rockville, MD

Workshop Goal and Objective

The purpose of this workshop was to bring together network researchers, operators, and application developers from national laboratories, academia, and industry to identify and discuss emerging opportunities and challenges in the design and development of a new generation of self-aware, self-organized, and self-protected network infrastructures to support emerging complex and hyper-connected open science environment of the future.

Workshop Co-chairs: Ian Foster/ANL, Thomas Lehman/UMD	
Breakout Topics	Organizers
Smart Network Architectures and Protocols	Tom Lehman/UMD/MAX, Bryan Lyles/ORNL, Inder Monger – ESnet/LBL
Applied AI-based Technologies for Smart Systems	Prasanna Balaprakash/ANL, Kalyan Perumalla, Nagi Rao/ORNL
Smart Cyber Defense in Open Science Environment	Stacy Prowell/ORNL
Intelligent Network-Intensive Scientific Workflows	Ian Foster/ANL, Raju Vatsavai/NCSU

Workshop Attendance ~ 70
- DOE Labs 23
- Academia: 38
- Other Agencies: 7

Workshop Report:
- Draft report: Mid January
- Final Report: Mid February

Other 2016 Workshops and Meetings

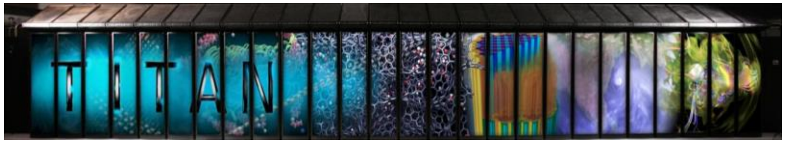
- Network Research Problems and Challenges for DOE Scientists Workshop (Feb. 1-2, 2016; Bethesda, MD) http://www.orau.gov/networkresearch2016/
- ASCR/HEP Quantum Sensors at the Intersections of Fundamental Science, QIS and Computing meeting (Feb. 25, 2016)
- STREAM 2016: Streaming Requirements, Experience, Applications And Middleware Workshop (March 22–23, 2016) http://www.orau.gov/streaming2016/
- X-Stack PI Meeting (April 5-7, 2016; LBNL) https://xstackwiki.modelado.org/April_6-7,_2016_-_X-Stack_PI_Meeting
- Emerging Technologies Program Review Meeting (April 14-15, 2016; San Francisco, CA)
- OS/R PI Meeting (May 23, 2016; Chicago, IL) https://xstackwiki.modelado.org/May_23,_2016_-_OS/R_PI_Meeting
- Computing Beyond 2025 Summit Meeting (Aug. 15-16, 2016)
- Quantum Testbeds Study Group (Aug. 23, 2016)
- Next Generation Networks for Science (NGNS) Principal Investigators' (PI) Meeting (Sept 8-9, 2016) http://www.orau.gov/ngns2016/default.htm
- Advances in Mathematical and Computational Climate Modeling Workshop (September 12–13, 2016) http://www.orau.gov/esmascr2016/
- Mathematical Multifaceted Integrated Capability Centers Summit (Nov. 1, 2016)
- Smart High-Performance Networks – Towards a New Generation of Intelligent Networking Infrastructure for Distributed Science Environment (Dec. 8-9, 2016) https://www.orau.gov/smarthp2016/default.htm

Facility and Project Updates

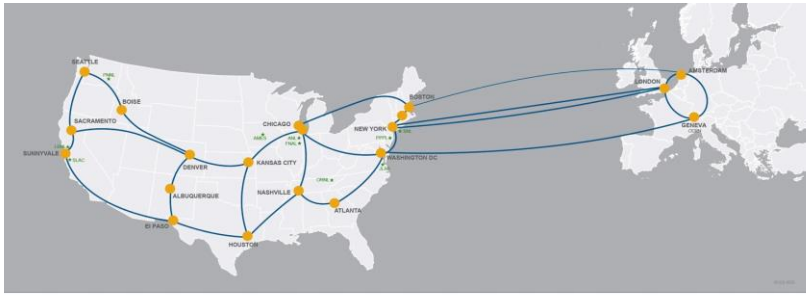
ASCR's Facilities

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)**

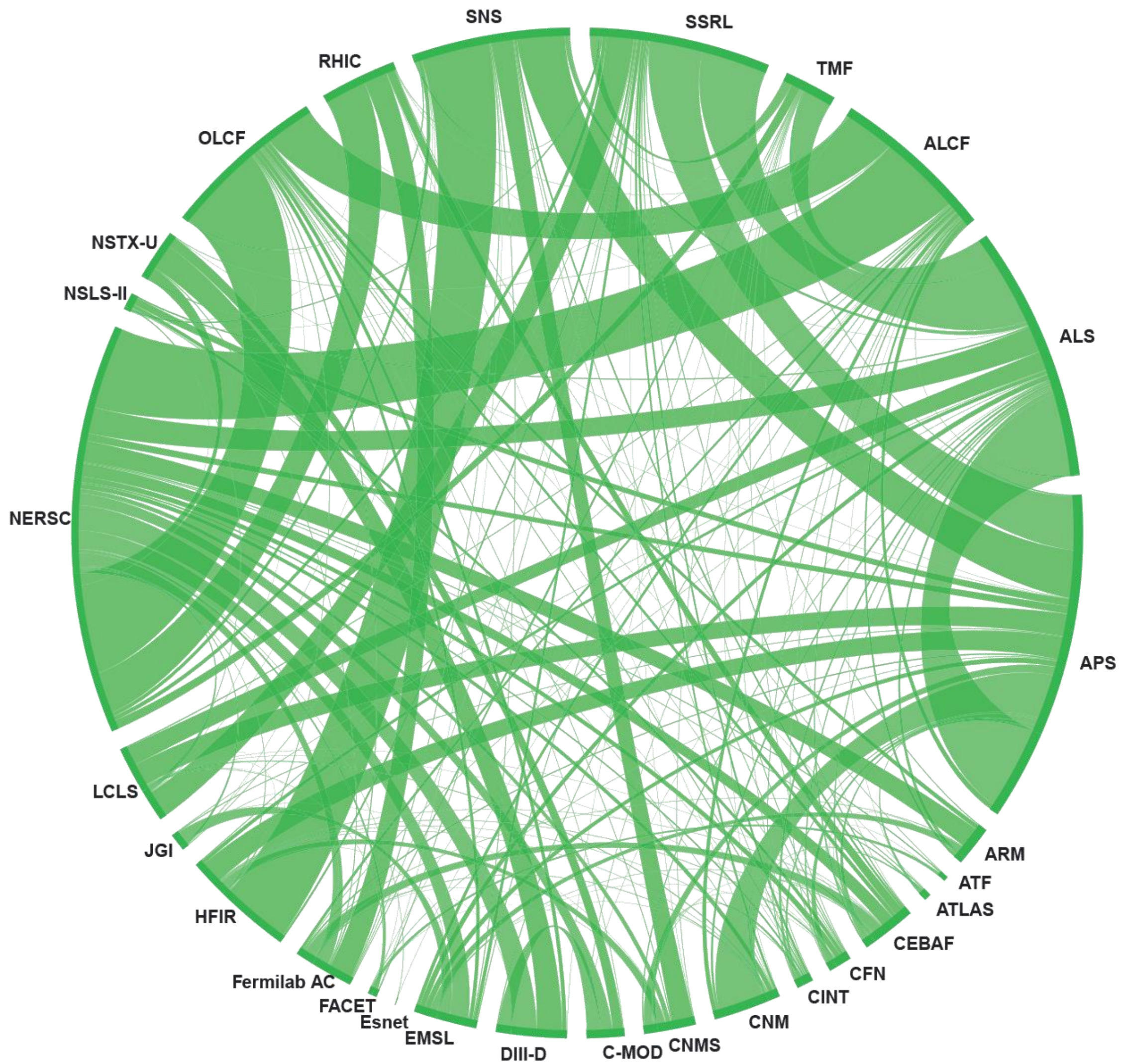
Path to the Future **– Research & Evaluation Prototypes**

ASCR Computing Upgrades At a Glance

System attributes	NERSC Now	OLCF Now	ALCF Now		NERSC Upgrade	OLCF Upgrade	ALCF Upgrades
Name Planned Installation	**Edison**	**TITAN**	**MIRA**	**Theta 2016**	**Cori 2016**	**Summit 2017-2018**	**Aurora 2018-2019**
System peak (PF)	2.6	27	10	>8.5	> 30	200	180
Peak Power (MW)	2	9	4.8	1.7	< 3.7	13.3	13
Total system memory	357 TB	710TB	768TB	>480 TB DDR4 + High Bandwidth Memory (HBM)	~1 PB DDR4 + High Bandwidth Memory (HBM)+1.5PB persistent memory	> 2.4 PB DDR4 + HBM + 3.7 PB persistent memory	> 7 PB High Bandwidth On-Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 3	> 40	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing Xeon Phi many core CPUs	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	>2,500 nodes	9,300 nodes 1,900 nodes in data partition	~4,600 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Aries	Dual Rail EDR-IB	2nd Generation Intel Omni-Path Architecture
File System	7.6 PB 168 GB/s, Lustre®	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS™	10PB, 210 GB/s Lustre initial	28 PB 744 GB/s Lustre®	120 PB 1 TB/s GPFS™	150 PB 1 TB/s Lustre®

User Crossover Among SC User Facilities, FY 2015

The width of the ribbon connecting two facilities corresponds to the number of users who utilized both of those facilities



NERSC-9 Project Description

- **Acquire and deploy a pre-exascale HPC system in 2020**
  - Serve the full range of SC research
  - Enable early exploration of concepts and technologies for future exascale systems
- **Some uncommon project features**
  - Alliance for Application Performance at Extreme Scale (APEX) partnership- NERSC and Alliance for Computing at Extreme Scale (ACES) (LANL and SNL)
  - Non-Recurring Engineering (NRE)
  - Lease-to-own financing (LTO)

- **CD-1/3a Alternative Selection and Initiate Procurements approved May 13, 2016**
  - Issue RFPs: Computing system, NRE, and Facility Upgrade (FE)
  - Appropriate to allow start of long-lead system procurement
  - Cost Range: \$65M - \$72M
  - CD-4: Q1 FY2023 (18 months of schedule contingency)

ESnet6 Mission Need / Capability Gap

- **Mission Need Statement**
  - Provide a network that addresses the next ten years of SC science requirements aligned with the facility vision to ensure that Scientific progress will be **completely unconstrained** by the physical location of instruments, people, computational resources, or data. "
  - **Objectives**
    - ***Capacity***
      - Handle exponential science data growth on network at reasonable cost, examples
    - ***Reliability and Resiliency***
      - Current network End of Life in 2019-2020 timeframe
      - Cyber-resiliency – protection against increasing level of cyber-security attacks
    - ***Flexibility***
      - Computing models changing with distributed multi-facility workflows ('superfacility') and needs for near real-time analysis with possibly streaming data from facilities

- **Critical Decision 0, Statement of Mission Need approved December 5, 2016**
  - ROM Cost Range: $58M - $99M
  - CD-4: FY2022, 12 months schedule contingency

ASCR Facilities | EXASCALE REQUIREMENTS REVIEWs

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

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.

SC Partner Program: Identify key computational science objectives from the Science Program that push exascale and describe the HPC ecosystem –HPC machine and related resources- needed to successfully accomplish your science goals

- Include continuum of computing needs from institution clusters to Leadership computing.
- Include modeling and simulation, scientific user facilities and data needs.

ASCR: Communicate 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 and SC Partner Programs.

Exascale Requirements Reviews

The Exascale Requirements Reviews brought together scientists, planners, and experts in each of the DOE's six Office of Science (SC) program offices:

- High-Energy Physics, June 2015
- Basic Energy Sciences, November 2015
- Fusion Energy Sciences, January 2016
- Biological and Environmental Science, March 2016
- Nuclear Physics, June 2016
- Advanced Scientific Computing Research, September 2016
- *Cross-Cut March 9-10 2017*

Path Forward

- **Nov 2016 – Feb 2017: Workshop reports completed. ASCR Centers collect and organize findings from reports and reviews.**
- **Feb – Mar 2017: ASCR Center's organize first-draft response to findings and shares with ASCR HQ**
  - Findings and responses include tags such as:
    - People – Center staff
    - Infrastructure – Software
    - Infrastructure – Hardware
    - In scope now
    - In scope but needs funding/recommended new scope
    - Out of scope for ASCR computing facility

Finding	Response
Finding 1	Response 1
Finding 2	Response 2

- **Mar 2017: Cross-cut workshop held**
- **Mar – June 2017: ASCR Centers write X-cut report. ASCR Centers and ASCR HQ iterate on findings and response**

Cross-cut – Computing, Data, Software, Training

- **Computing**
  - Allocations, Access, Policies
    - ASCR, BER, FES, HEP, NP
  - Hardware
    - We have mission-need-scale requirements
      - *BER,* BES, FES, HEP, NP
    - Substantial requirements for computational complexity in a wider range of use models
    - Improved balance of coming systems (BW)
      - FES, NP
    - More available testbeds
      - ASCR, BER
- **Training & Workforce Development**
  - Collaborations
    - BES, FES, HEP, NP
  - Training for current and next generation systems
    - BES, FES, NP
  - Workforce
    - ASCR, BER, BES, FES, HEP, NP

Cross-cut – Computing, Data, Software, Training

- **Software Requirements**
  - Workflows - HEP, FES, NP
    - Large ensembles, local and remote
    - Provenance and metadata
    - Coupling with experiment
    - Smoother integration of resources
  - Models/Methods/Algorithms – ASCR, BER, BES, FES, NP
  - Common Environment – ASCR, BER, BES, FES, HEP, NP
  - Portability & Performance – ASCR, FES, HEP, NP
  - Reducing Programming Complexity – FES
- **Data**
  - Multi-site experimental and simulation workflows – ASCR, BER, BES, FES, HEP, NP
  - Large-Scale Data Analysis – ASCR, BER, BES, FES, HEP, NP
  - Data Volume and Velocity – ASCR, FES, HEP, NP
  - Metadata and Provenance – FES
  - Long-Term Data Curation – ASCR, BES, NP
  - *ASCR has a lot of requirements here, but a very different nature*

Current plans for Cross cut

- **Planned Meeting Items:**
  - ASCR Center’s share summary findings with community for input
  - ASCR Center’s highlight to community requirements that are cross-cutting
  - SC Scientists from diverse technical backgrounds come together as a community and interact on common technical challenges and needs
- **Planned Meeting Products:**
  - Refined and community vetted set of findings
  - X-cut workshop report of high level findings across 6 reports and summary findings of particular areas of importance across the office of science

Exascale

Exascale Background: Components of the DOE Exascale Program

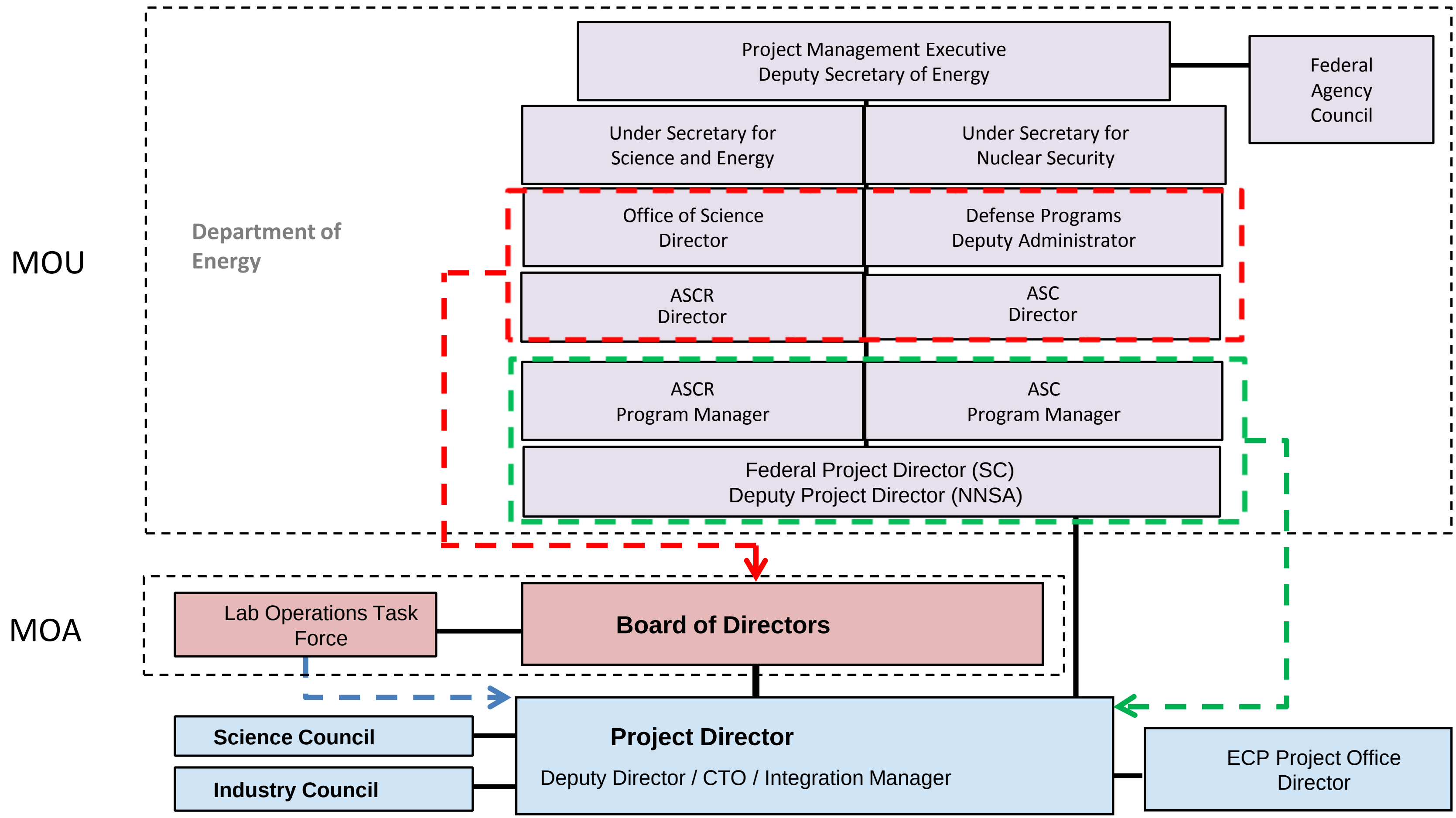
- **Exascale Computing Initiative (ECI) Crosscut**
  - Even though NNSA and SC had been collaborating on Exascale since 2009, the ECI crosscut was initiated in FY 2016 to support research, development, and computer-system procurements to deliver an exascale (10^{18} ops/sec) computing capability by the mid-2020s.
  - It is a partnership between SC and NNSA, addressing science and national security missions, but also includes investments in software application developments in both SC (BES and BER) and NNSA.

- **Exascale Computing Project (ECP)**
  - ECP project started in FY2016 with the establishment of a project office at Oak Ridge and is being managed according to the principles of DOE Order 413.3B.
  - Beginning with the FY 2017 appropriation, the ASCR Exascale funding will transition into the ASCR budget as a separate line item, SC-ECP, and be
  - ECP is has four focus areas: Application Development, Software Technology, Hardware Technology and Exascale Systems.

ECP update

- The DOE exascale effort has been underway since 2009, a partnership between Office of Science (SC) and NNSA
  - Exascale was identified as an objective in the National Strategic Computing Initiative (NSCI) Executive Order in 2015
  - In FY 2016, the Exascale Computing Project (ECP) office was established in Oak Ridge and a management team selected to manage the research, development, and delivery of capable exascale architectures by the mid-2020s
  - The actual Exascale systems will be deployed by the laboratories/facilities that will operate them.
- The Exascale Mission Need Statement was jointly approved by the Office of Science and NNSA on April 14, 2016
- Critical Decision-0, *Approve Mission Need*, was approved by the Secretary's Energy Science Acquisition Approval Board (ESAAB) and the Deputy Secretary as the Project Mangement Executive on July 28, 2016,
  - ROM Cost Range: $3.1 Billion - $5.1 Billion
  - Project completion in 2026 (which includes 12 months of schedule contingency)
- Critical Decision-1 *Alternative Selection and Cost Range* and Critical Decision 3A *Long Lead Procurement (LLP) for Hardware and Software Technology Research and Development with vendors and Test Beds* was approved by the ESAAB and we are waiting for the Deputy Secretary's signature
  - ROM Cost Range: $3.5 Billion - $5.7 Billion
  - Project completion in 2023 (which includes 12 months of schedule contingency)

ECP Project Organization



Dashed lines represent lines of communication

ECP External Governing Documents

- **MOU** between DOE/SC and NNSA/DP updated to define roles and responsibilities of the Programs responsible for the Exascale Computing Initiative which includes the Exascale Computing Project, signed November 23, 2016

- **MOA** between the six national laboratories (ANL, LANL, LBNL, LLNL, ORNL and SNL) responsible for executing the research, development and deployment of the exascale computing project signed by the laboratory directors on August 3, 2016
  - The ECP project office (ECPO) resides at ORNL and the ORNL Lab Director will maintain oversight of all ECPO operations including oversight of the ECP Project Director (PD) regarding the ECPO.
  - The ECP Board of Directors will be composed of an executive committee (EC) comprised of the laboratory directors from each core partner laboratory and 3 external members and meet at least twice per year; the Board Chair will be elected from the SC lab members.
  - The EC hires the ECP Project Director who serves at the discretion of the board
  - The EC will establish a standing Laboratory Operations Task Force (LOTF) comprised of one delegate from each partner laboratory who will have the management responsibility at their laboratory for the resources needed by the ECP project. The LOTF will meet bi-weekly with the PD to discuss staffing, operational and management issues.

Paul Messina's Update will provide more information on ECP

FY 2017 Updates

SciDAC FOA/LAB status

FOA/LAB *PM*	1697* HEP *Lali Chatterjee*	1681* BER: Coupled Systems *Dorothy Koch*	1682 BER: Pilot Projects *Dorothy Koch*	1698 NP *Ted Barnes*	1670 FES *John Mandrekas*	1674 NE *Dan Funk*
Posted	4 Nov 2016	4 Nov 2016	9 Nov 2016	10 Nov 2016	16 Nov 2016	16 Dec 2016
LOI/ Pre-Proposal	17 Jan 2017	17 Jan 2017	17 Jan 2017	16 Dec 2016	9 Jan 2017	15 Feb 2017
Proposal due	**27 Feb 2017**	**15 Mar 2017**	**15 Mar 2017**	**24 Feb 2017**	**21 Feb 2017**	**5 Apr 2017**
Total Funding (years)	$25M (5)	$35M (5)	$15.8M (2.5)	$25M (5)	$90M (5)	$7.5M (5)

*LAB Announcement only

Upcoming SciDAC-4 Institutes FOA is planned to be released in late Spring 2017.

SciDAC: Partnership with the Office of Nuclear Energy

FOA/LAB 17-1674 from ASCR & NE is open to Labs, University, & Industry

Background

- ASCR & NE funded an 18-month Pilot Project (via Open Call) in FY2016
  - Led by UT-K (Brian Wirth) in collaboration w/ ORNL, PNNL, LANL, & INL
  - Engages experts from FASTMath and SUPER SciDAC-3 Institutes
- Dan Funk (NE-51) has been participating as a Partner PM in SciDAC PM meetings

Topic focused on modeling & simulation of nuclear fuels via HPC

Predict microstructure evolution in current and advanced nuclear fuel and cladding by leveraging DOE-HPC capabilities & applied math/CS expertise

Timeline (FY2017)

- Published 16 Dec. 2016, LOIs due 15 Feb. 2017, Proposals due 5 Apr. 2017
- Awards to be made by late June 2017, likely for one multi-institutional project

Quantum Testbed Stakeholder Workshop

In Feb. 2017, ASCR will bring key stakeholder groups together to:

- identify individual capabilities and interests in quantum computing hardware and its use for science applications
- share best practices for management of collaborative research facilities, including topics such as workforce training and building strong relationships with the research community
- identify technology that will be important for the success of a testbed facility with the goal of advancing quantum computing for scientific applications in the next five years

Agenda to include:

- Presentations outlining DOE lab capabilities
- Breakout discussions on topics including user community development, workforce training, quantum co-design, technical challenges
- Discussion with industry to identify synergistic activities across the national quantum ecosystem

Workshop Dates: Feb. 14-16, 2017

Location: Washington, D.C.

White Papers Due: Jan. 5, 2017

Website: https://www.orau.gov/qtsws/default.htm

2017 AFRL-DOE Energy Consequences of Information (ECI) Workshop

- When and Where: February 23-25, 2017, Santa Fe, NM
- The Air Force Research Laboratory (AFRL), the Air Force Office of Scientific Research (AFOSR), and the Department of Energy (DOE) Office of Advanced Scientific Computing Research (ASCR) are sponsoring a workshop on the Energy Consequences of Information Processing.
- The main goal of the workshop will be to bring together leaders from national laboratories, industry, academia, and government for the purpose of examining crucial challenges, including runaway costs at high performance computing centers and the ever increasing demands for computation in energy constrained environments, assessing the current state of the art in both fundamental understanding and in technology, and developing recommendations for future collaborations.

https://community.apan.org/wg/afosr/w/researchareas/18305.2017-energy-consequences-of-information-eci/

Other Planned Workshops or Summits

- **Summit on Correctness for Exascale and Beyond (Winter 2017)**
- **UQ for Coupled and Networked Systems – ~Feb 1, 2016**
- **SciDAC-3 Institutes-Manufacturing Innovation Institutes Summit (February 2017)**
- **Network Debugging and Troubleshooting (Spring 2017)**
- **Distributed Workflow Simulations (Spring 2017)**
- **Workshop on HPC Correctness (Spring 2017)**
- **BRAIN (Spring 2017)**
- **ASCR/BER Study Group on collaboration with ACME (Late Spring 2017)-**
- **Workshop on Software Stack for Data Convergence (June 2017)**
- **Hypothesis Generation & Validation Summit (Early Summer 2017)**
- **Network Debugging and Troubleshooting (Summer 2017)**
- **Real-Time Data Analytics Summit (Q3 2017)**
- **Probabilistic Computing Summit (Fall 2017)**
- **Provenance Workshop (Fall, 2017)**
- **Mathematics for Emerging Technologies: Approximate Computing for power-optimized simulation at scale (September 2017)**
- **Post-digital communications (All-Optical Networks) (FY17 -TBD)**
- **Open science software stack for mini/Micro clouds (FY17 – TBD)**
- **Smart systems and application to open science (FY17 – TBD)**

ASCR at a Glance

Office of Advanced Scientific Computing Research

Acting Associate Director – Barbara Helland
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 – Christine Chalk
Phone: 301-903-9958
E-mail: Barbara.Helland@science.doe.gov

Relevant Websites

ASCR: science.energy.gov/ascr/

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 COV Charge

Department of Energy
Office of Science
Washington, DC 20585

Professor Daniel A. Reed, Chair of the ASCAC
Office of the Vice President for Research and Economic Development
University of Iowa
2660 UCC
Iowa City, Iowa 52242

Dear Professor Reed:

Thank you for the excellent Committee of Visitors (COV) review of the Next Generation Networking for Science program. Your report recommendations are helping us to improve the management of this important program.

To help the research communities utilize the capabilities of current and future supercomputers, the Advanced Scientific Computing Research program supports basic research programs in Applied Mathematics, Computer Science, Computational Partnerships called Scientific Discovery through Advanced Computing or SciDAC, and Next Generation Networking for Science. To ensure the integrity of this research program and to ensure that it is meeting the challenges of the DOE mission, I am asking the Advanced Scientific Computing Advisory Committee (ASCAC) to assemble a Committee of Visitors to review the management processes for the ASCR research portfolio. As this portfolio includes scientific applications supported by the other programs across the Office of Science and representing a wide array of disciplines, you may wish to have a larger committee than is usual for an ASCAC COV. A report will be expected at the Fall 2017 ASCAC meeting.

The COV should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. The panel should assess the operations of the Division's program elements during the fiscal years 2013, 2014, and 2015. The panel may examine any files from this period for both DOE laboratory projects and university projects. The Committee will be provided with background material on the program prior to the meeting.

I would like the Committee to consider and provide their evaluation of the following two major program elements:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
   (a) solicit, review, recommend, and document proposal actions, and
   (b) monitor active projects and programs.