DOE Office of Advanced Scientific Computing Research

Presented to the

Advanced Scientific Computing Advisory Committee

by

Steve Binkley
Associate Director

April 4, 2016

Some Agenda Details

- **UPDATE ON THE EXASCALE COMPUTING PROJECT**
  - *Paul Messina, ECP Director*
- **NNSA INVESTIGATION OF ADVANCED PROGRAMMING MODELS AND RUNTIME SYSTEMS FOR EXASCALE**
  - *Pat McCormick, Los Alamos National Laboratory*
- **NEUROMORPHIC COMPUTING**
  - *Robinson Pino, ASCR*
- **ADVANCED COMPUTING TECH TEAM (ACTT)**
  - *Michael Martin, ASCR*

- **QUANTUM COMPUTING / QUANTUM INFORMATION SCIENCE**
  - *Steve Binkley*
- **THE BRAIN INITIATIVE AND DOE-NCI PILOT PROJECTS**
  - *Rick Stevens, Argonne National Laboratory*
- **SC LAB PLANNING**
  - *Barbara Helland, ASCR*
- **COMPUTING RESEARCH LEADERSHIP COUNCIL**
  - *David Brown, Lawrence Berkeley National Laboratory*

FY 2017 Budget

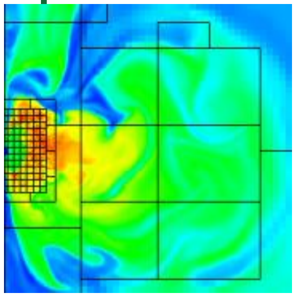
Office of Science FY 2017 Budget Request to Congress

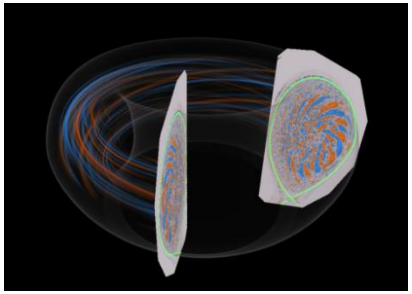
(Dollars in thousands)

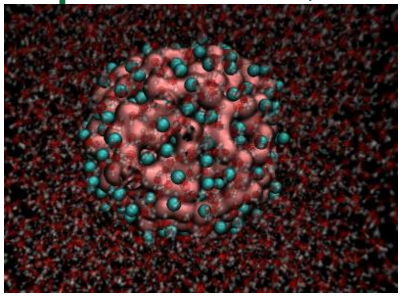
	FY 2015 Enacted Approp.	FY 2015 Current Approp.	FY 2016 Enacted Approp.	FY 2017 President's Request	FY 2017 President's Req. vs. FY 2016 Enacted Approp.	
Science						
Advanced Scientific Computing Research	541,000	523,411	621,000	663,180	+42,180	+6.8%
Basic Energy Sciences	1,733,200	1,682,924	1,849,000	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%**

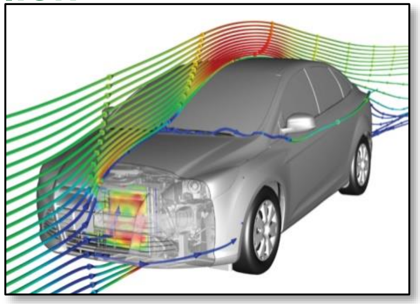
ASCR FY 2017 Budget Highlights

- **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 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

	FY 2015 Enacted Approp.	FY 2015 Current Approp.	FY 2016 President's Request	FY 2016 Enacted Approp.	FY 2017 President's Request	FY 2017 President's Req. vs. FY 2016 Enacted Approp.	
Mathematical, Computational, and Computer Sciences Research							
Applied Mathematics	49,155	49,454	49,229	49,229	39,229	-10,000	-20.3%
Exascale	*(5,000)*	*(5,000)*	*(5,000)*	*(10,000)*	*(…)*	*(-10,000)*	*(-100.0%)*
Computer Science	55,767	55,259	56,842	56,848	39,296	-17,552	-30.9%
Exascale	*(20,000)*	*(20,000)*	*(25,106)*	*(20,423)*	*(…)*	*(-20,423)*	*(-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%**

Components of the Exascale Program

- Exascale Computing Initiative (ECI)
  - The ECI 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.
  - The Exascale Crosscut includes primary investments by SC/ASCR and NNSA/ASC and software application developments in both SC (BES and BER) and NNSA.

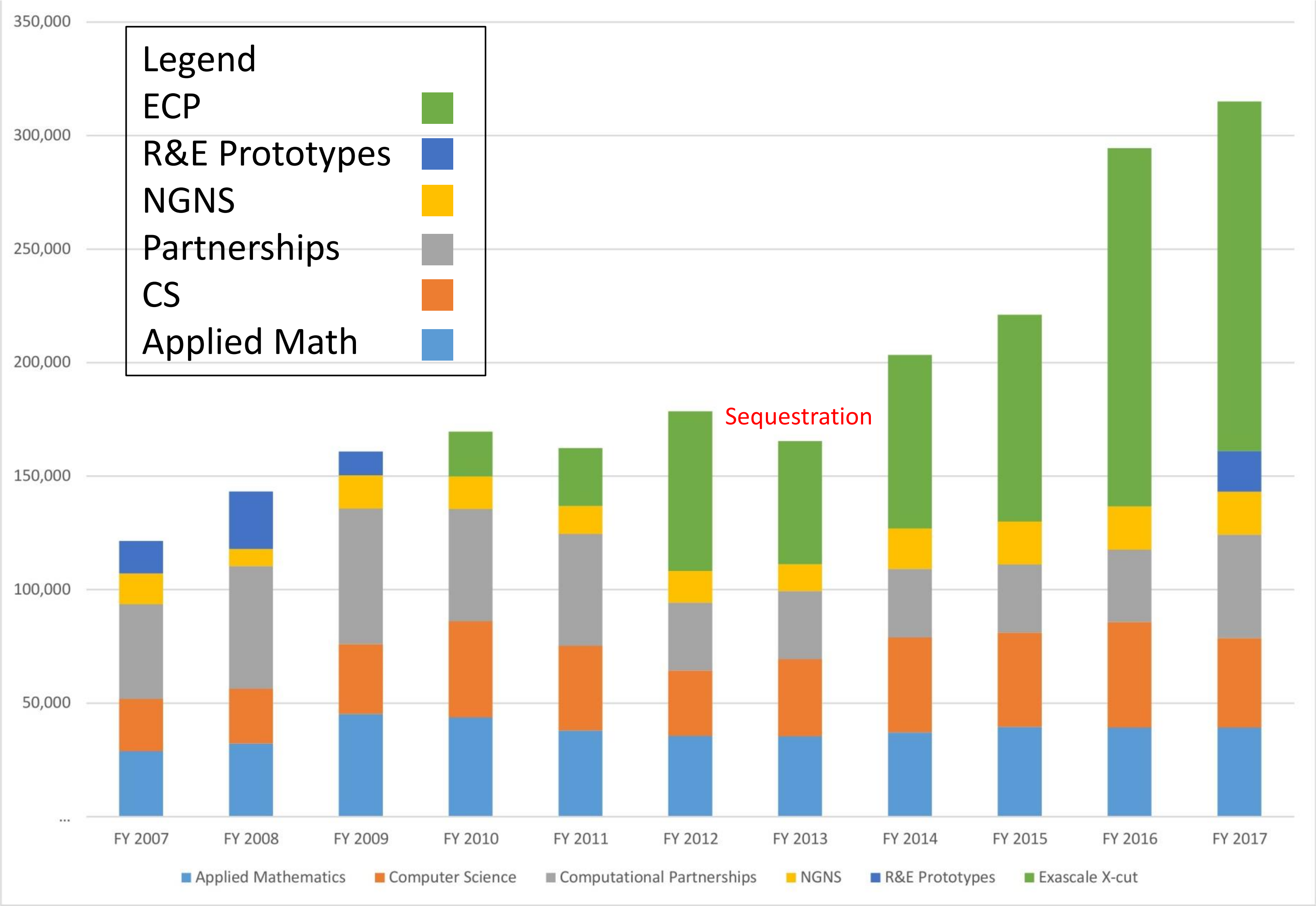
- Exascale Computing Project (ECP)
  - Beginning in FY 2017, the ASCR ECI funding is transitioned to the DOE project (the ECP), which is managed according to the principles of DOE Order 413.3b.
  - First four years focus on research in software (new algorithms and methods to support application and system software development) and hardware (node and system design), followed by acquisition of systems
  - The new ECP subprogram in ASCR (SC-ECP) includes only activities required for the delivery of the exascale computers. An ECP Project Office has been established ORNL.
  - NNSA/ASC Advanced Technology Development and Mitigation (ATDM) supports activities for the delivery of exascale computers and the development of applications.

FY 2017 Exascale Crosscut

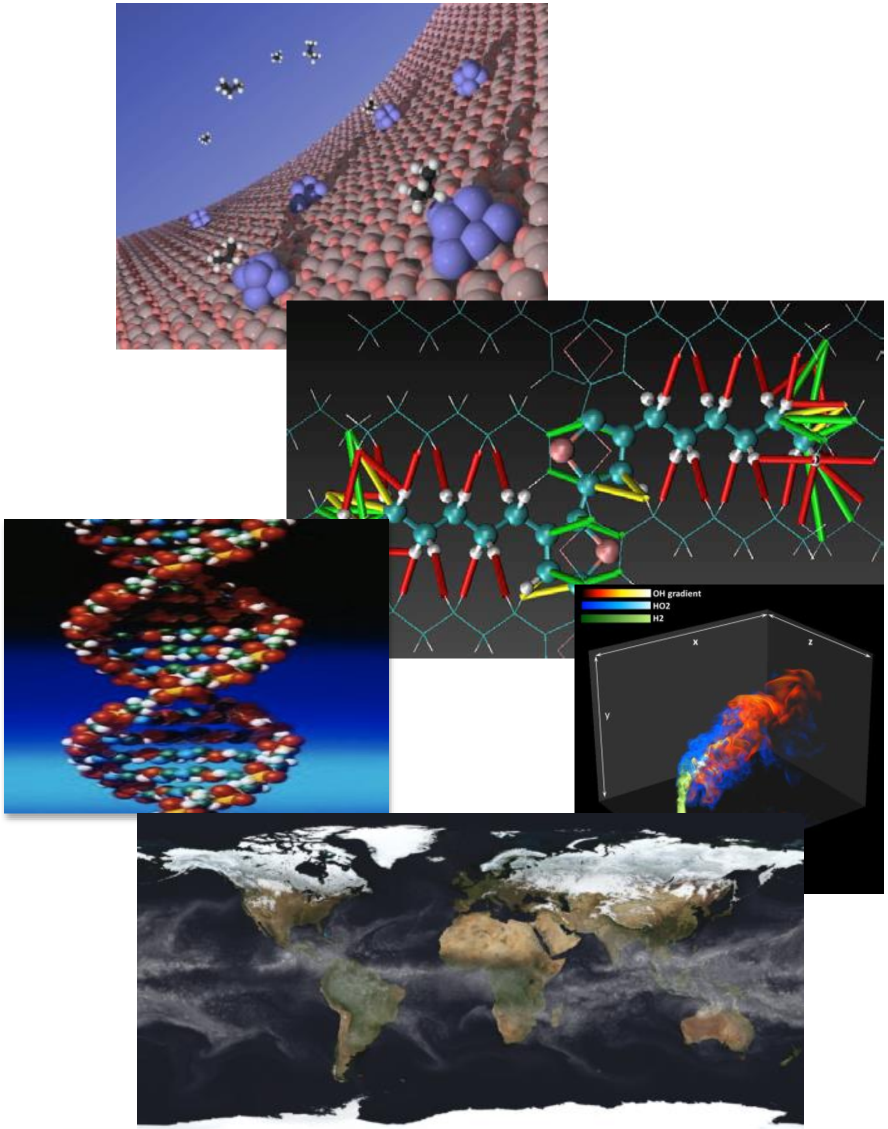
Exascale Initiative Starts

	FY 2012 Actuals	FY 2013 Actuals	FY 2014 Actuals	FY 2015 Enacted	FY2016 Enacted	FY2017 Request
NNSA						
ASC: Advanced Technology Development and Mitigation	30,500	29,600	42,400	50,000	64,000	95,000
NNSA Total				**50,000**	**64,000**	**95,000**
SC						
ASCR Total	70,300	54,900	77,500	91,000	157,894	154,000
BER				0	18,730	10,000
BES				8,000	12,000	26,000
SC Total				**99,000**	**188,600**	**190,000**
Exascale Total	**100,800**	**84,500**	**119,900**	**149,000**	**252,600**	**285,000**

Historical Exascale Funding



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 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**

Staffing Changes

ASCR Staffing – New Program Manager

Claire E. Cramer

Program Manager in ASCR Research & Evaluation Prototypes area.
Focus on Future Computing Technologies.

- EDUCATION
  - UNIVERSITY OF WASHINGTON, Ph.D., Physics
  - BROWN UNIVERSITY, Sc.B., Physics
- EXPERIENCE
  - NATIONAL SCIENCE AND TECHNOLOGY COUNCIL
    - *Executive Secretary, Interagency Working Group in Quantum Information Science*
  - NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
    - *Physicist, Physical Measurement Laboratory*
  - NATIONAL SCIENCE FOUNDATION
    - *Program Officer (detail), Astronomy Division*
  - OFFICE OF MANAGEMENT AND BUDGET
    - *Budget Examiner (detail), Energy Branch*
  - SMITHSONIAN ASTROPHYSICAL OBSERVATORY, Education Specialist
  - HARVARD UNIVERSITY, Postdoctoral Fellow
  - U.S. PEACE CORPS

Facilities Status

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**	**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 + High Bandwidth Memory (HBM)+1.5PB persistent memory	**> 2.4 PB DDR4 + HBM + 3.7 PB persistent memory**	>480 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On-Package Memory 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**	>2,500 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	**Dual Rail EDR-IB**	Aries	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™	28 PB 744 GB/s Lustre®	**120 PB 1 TB/s GPFS™**	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre®

U.S. DEPARTMENT OF ENERGY

FY 2017 Updates

Details of Mission Innovation

- **Mission Innovation** includes twenty countries that have committed to double their respective clean energy R&D investment over five years, including the top five most populous nations – China, India, the United States, Indonesia, and Brazil.

- Mission Innovation is complemented by a separate private sector-led effort, called the **Breakthrough Energy Coalition (BEC)**, which has pledged to invest private capital in clean energy, focusing on early-stage innovations. Spearheaded by Bill Gates, the BEC includes over 28 private capital investors from 10 countries.

- BEC describes its role as that of "…a different kind of private investor with a long term commitment to new technologies who is willing to put truly patient flexible risk capital to work."

- Within DOE, new funding in FY 2017 for Mission Innovation will be strategically focused on early stage research and development, which offers the greatest opportunity for breakthroughs and transformative changes and has proven to yield the highest return on investment.

Mission Innovation Participating Countries

- Australia
- Brazil
- Canada
- Chile
- China
- Denmark
- France
- Germany
- India
- Indonesia
- Italy
- Japan
- Mexico
- Norway
- Saudi Arabia
- South Korea
- Sweden
- United Arab Emirates
- United Kingdom
- United States

Office of Science Investments for Mission Innovation

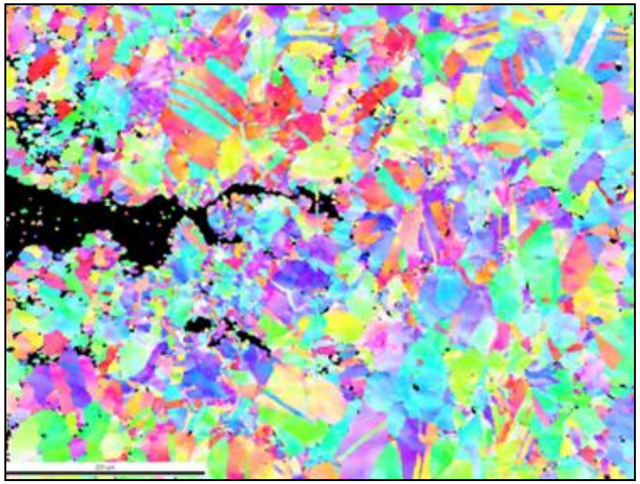
$100M in new funding in FY 2017

ASCR (+$10M)

- Computational Partnerships with EFRCs on solar, CO_2 reduction, catalysis, storage, subsurface, and biofuels; possibly new partnerships in wind and nuclear ($10M)

BES (+$51M)

- Energy Efficiency: Catalysts, modeled after nature's enzymes, that can operate at low-temperature and under ambient conditions; lightweight metallic materials; thermocaloric materials ($34.4M)
- Materials for Clean Energy: Self-healing materials for corrosive and high radiation environments (next-gen corrosive-resistant materials based on experiments and multi-scale modeling; chemistry under harsh or extreme environments) ($16.6M)



Analysis of cracks at the nanoscale

BER (+$35M)

- Biosystems design (computationally design and then bio-engineer biosystems) to introduce beneficial traits into plants and microbes for clean energy applications ($20M)
- Bioenergy Research Centers: New investments to translate 10 years of BRC research to industry ($15M, $5M per BRC)

FES (+4M)

- Whole-device fusion modeling and simulation using SciDAC partnerships ($4M)

SC Contributions to the BRAIN Initiative

- In FY 2017, ASCR, BER, and BES are partnering with NIH on the BRAIN initiative
  - ASCR ($3M) – HPC, data management, computational science
  - BES ($4M) – X-ray light sources and Nanoscale Science Research Centers for brain imaging and sensing, including fabricating biocompatible electronic materials and sensors
  - BER ($2M) – Joint Genome Institute and Environmental Molecular Science Laboratory to enable biosensor synthesis and characterization

Brain Research through Advancing Innovative Neurotechnologies

- SC Scientific User Facilities will help develop:
  - High-resolution tools for measuring neurological processes
  - Dynamic, real-time read-out of neurological measurements
  - Computational frameworks for analyzing and using the multi-modal data.
- A Joint DOE-NIH BRAIN Workshop (October 2015) defined the scope of DOE participation.

Post-Moore's Law Computing: What comes after exascale?

- CMOS lithographic feature sizes are approaching fundamental limits
  - Currently at 14 nm (both Intel and Nvidia)
  - 10 nm is projected for 2016 (both Intel and Nvidia)
    - However, gate lengths may be smaller than 6 nm – corresponding gate dielectric thickness may reach a monolayer or less
  - The industry roadmap reaches beyond 10 nm (7 nm and 5 nm) but may be unattainable
    - Non-silicon extensions of CMOS, e.g., using III-V materials or nanotubes/nanowires or non-CMOS technologies, including molecular electronics, spin-based computing, single-electron devices, and graphene have been proposed
    - At scales of ~7-5 nm, quantum tunneling may become significant
  - Capital costs for tooling are increasing dramatically as feature sizes shrink
- Options:
  - Computing using superconducting technologies
  - Quantum computing/quantum information science
  - Neuromorphic computing
  - Probabilistic computing
  - ???

Considerable R&D required

Research and Evaluation Prototypes
Quantum Computing: Testbeds

- **Challenge:**

  A major barrier to developing quantum computing is availability of testbed computing systems that can be used to explore algorithms and computational approaches

- **FY 2017 Objective:**

  Initiate the development of two to three testbeds, which would support ASCR, BES, and HEP-based algorithm development activities. These testbeds will not look like conventional computers – they would likely comprise approximately a six-nine qubits and likely would be based on optical or circuit-based approaches, requiring modest technical support to use.

Computational Partnerships
Quantum Computing: Algorithms

- ## Challenge:

  Research community workshops have identified scientific applications that are important to DOE missions (both SC and NNSA) that can be attacked using quantum algorithms.

- ## FY 2017 Objective:

  Initiate two EFRC-sized efforts, focused on problems relevant to SC, to begin development of quantum algorithms and to evaluate efficacy of this funding modality for achieving the needed multidisciplinary integration. These EFRC-like activities would use the quantum testbeds in a co-design fashion, feeding back into the testbeds ideas for improvement.

Research and Evaluation Prototypes Cyber Security for Scientific Integrity

- **Challenge:**

  Given the increasing threat from cyber-attacks on federal resources and the expertise within the ASCR research community, ASCR will initiate a modest research effort in cybersecurity in FY 2017 with an emphasis on the unique challenges of the Department's HPC facilities, which are not currently addressed by ongoing cyber-security R&D.

- **FY 2017 Objectives:**
  - Research community workshops have identified transformative tools and techniques to address HPC cybersecurity challenges affecting scientific integrity and basic research
  - Establish cybersecurity ASCR team with members from our federal workforce, scientific laboratory facilities, and/or talented individuals from other agencies, academia, or industry
  - Understand the challenge and plan scientific integrity and cybersecurity-focused risk analysis deep dives across SC supercomputer facilities and ESnet
  - Establish communication strategy and share of information that is unique to SC scientific facilities

ASCR at a Glance

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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?