U.S. DEPARTMENT OF ENERGY

DOE Office of Advanced Scientific Computing Research

Presented to the
Advanced Scientific Computing Advisory Committee

by

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Associate Director

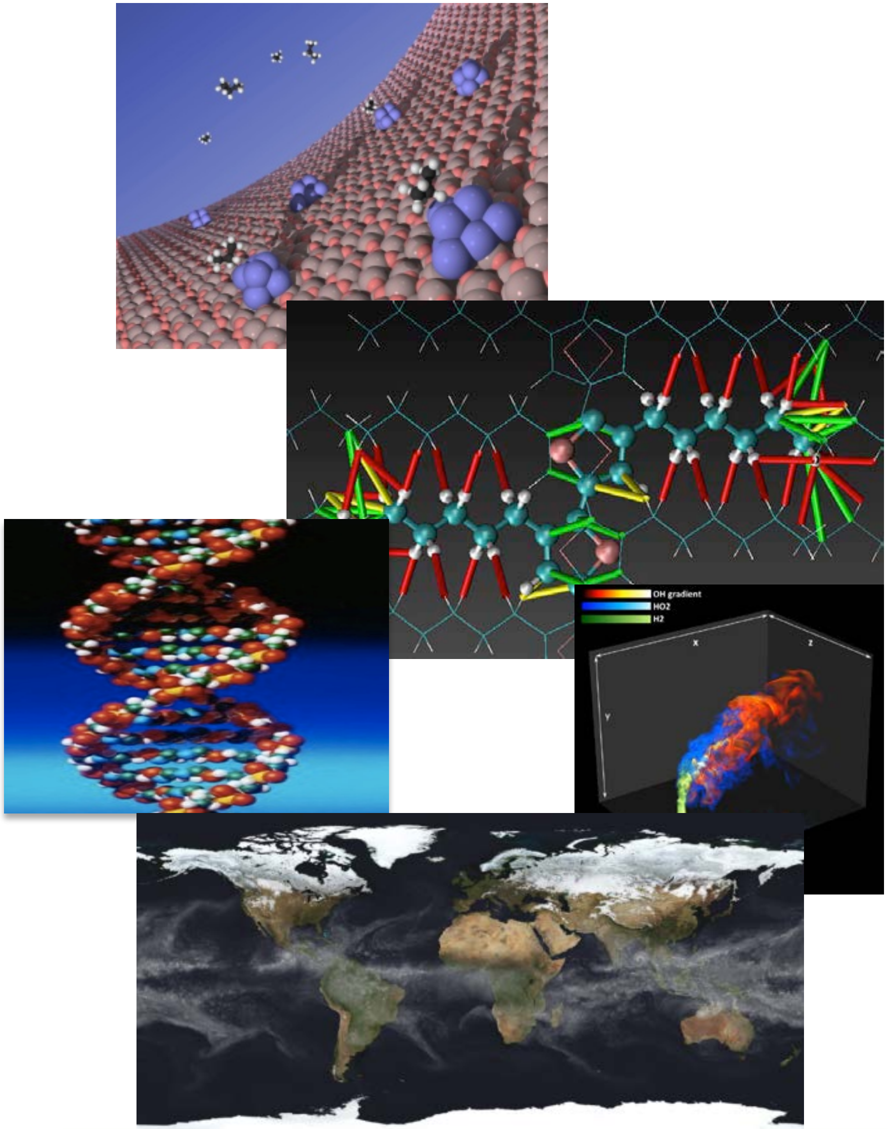
March 31, 2014

Budget

Office of Science FY 2015 Budget Request to Congress
(Dollars in thousands)

	FY 2013 Current (prior to SBIR/STTR)	FY 2013 Current Approp.	FY 2014 Enacted Approp.	FY 2015 President's Request	FY15 President's Request vs. FY14 Enacted Approp.	
Advanced Scientific Computing Research	417,778	405,000	478,093	541,000	+62,907	+13.2%
Basic Energy Sciences	1,596,166	1,551,256	1,711,929	1,806,500	+94,571	+5.5%
Biological and Environmental Research	578,294	560,657	609,696	628,000	+18,304	+3.0%
Fusion Energy Sciences	385,137	377,776	504,677	416,000	-88,677	-17.6%
High Energy Physics	748,314	727,523	796,521	744,000	-52,521	-6.6%
Nuclear Physics	519,859	507,248	569,138	593,573	+24,435	+4.3%
Workforce Development for Teachers and Scientists	17,486	17,486	26,500	19,500	-7,000	-26.4%
Science Laboratories Infrastructure	105,673	105,673	97,818	79,189	-18,629	-19.0%
Safeguards and Security	77,506	77,506	87,000	94,000	+7,000	+8.0%
Program Direction	174,862	174,862	185,000	189,393	+4,393	+2.4%
Subtotal, Office of Science	**4,621,075**	**4,504,987**	**5,066,372**	**5,111,155**	+44,783	+0.9%
Small Business Innovation Research/Technology Transfer	...	176,208	...	...	...	...
Use of Prior Year Balances	...	...	...	...	...	...
Total, Office of Science	**4,621,075**	**4,681,195**	**5,066,372**	**5,111,155**	+44,783	+0.9%

FY 2015 ASCR Budget Priorities



- **Investment Priorities**
  - **C**onduct research and development, and design efforts in hardware software, and mathematical technologies that will produce exascale systems in 2022.
  - **P**repare today's scientific and data-intensive computing applications to migrate to and take full advantage of emerging technologies from research, development and design efforts.
  - **A**cquire and operate more capable computing systems, from multi-petaflop through exascale computing systems that incorporate technologies emerging from research investments.

ASCR Budget Overview

		FY 2013 Current Approp. (prior to SBIR/STTR)	FY 2014 Enacted Approp.	FY 2015 President's Request	*FY15 vs. FY14*
	Advanced Scientific Computing Research				
Exascale, Data	Applied Mathematics	43,341	49,500	52,155	*+2,655*
Exascale, Data	Computer Science	44,299	54,580	58,267	*+3,687*
Exascale, Data	Computational Partnerships (SciDAC)	41,971	46,918	46,918	*+0*
Data	Next Generation Networking for Science	11,779	15,931	19,500	*+3,569*
	SBIR/STTR	4,924	5,518	6,035	*+517*
	Total, Mathematical, Computational, and Computer Sciences Research	*146,314*	*172,447*	*182,875*	*+10,428*
	High Performance Production Computing (NERSC)	62,000	65,605	69,000	+3,395
	Leadership Computing Facilities	146,000	160,000	184,637	+24,637
Exascale	Research and Evaluation Prototypes	24,000	37,784	57,934	+20,150
Data	High Performance Network Facilities and Testbeds (ESnet)	31,610	32,608	35,000	+2,392
	SBIR/STTR	7,854	9,649	11,554	+1,905
	Total, High Performance Computing and Network Facilities	*271,464*	*305,646*	*358,125*	*+52,479*
	Total, Advanced Scientific Computing Research	**417,778**	**478,093**	**541,000**	***+62,907***

ASCR FY 2015 Budget Highlights* ($K)

- **Exascale *Crosscut*** **91,000†**

  Continue strategic investments to address the challenges of the next generation of computing to ensure that DOE applications continue to efficiently harness the potential of commercial hardware.

- **Data Intensive Science *Increase*** **+9,911**

  Continue building a portfolio of research investments that address the specific challenges from the massive data expected from DOE mission research, including research at current and planned DOE scientific user facilities and research to develop novel mathematical analysis techniques to understand and extract meaning from these massive datasets.

- **Facilities *Increase*** **+30,424**

  Begin preparations for 75-200 petaflop upgrades at each Leadership computing facility; support move of NERSC resources into the new Computational Research and Theory building, expansion of ESnet to support SC facilities and experiments in the US and Europe and creation of a Computational Science Post Doctoral Training program at the LCF's and NERSC.

* Excludes increases in SBIR

† FY 2014 crosscut for Exascale was $76,364K

Updates

(activities affecting ASCR)

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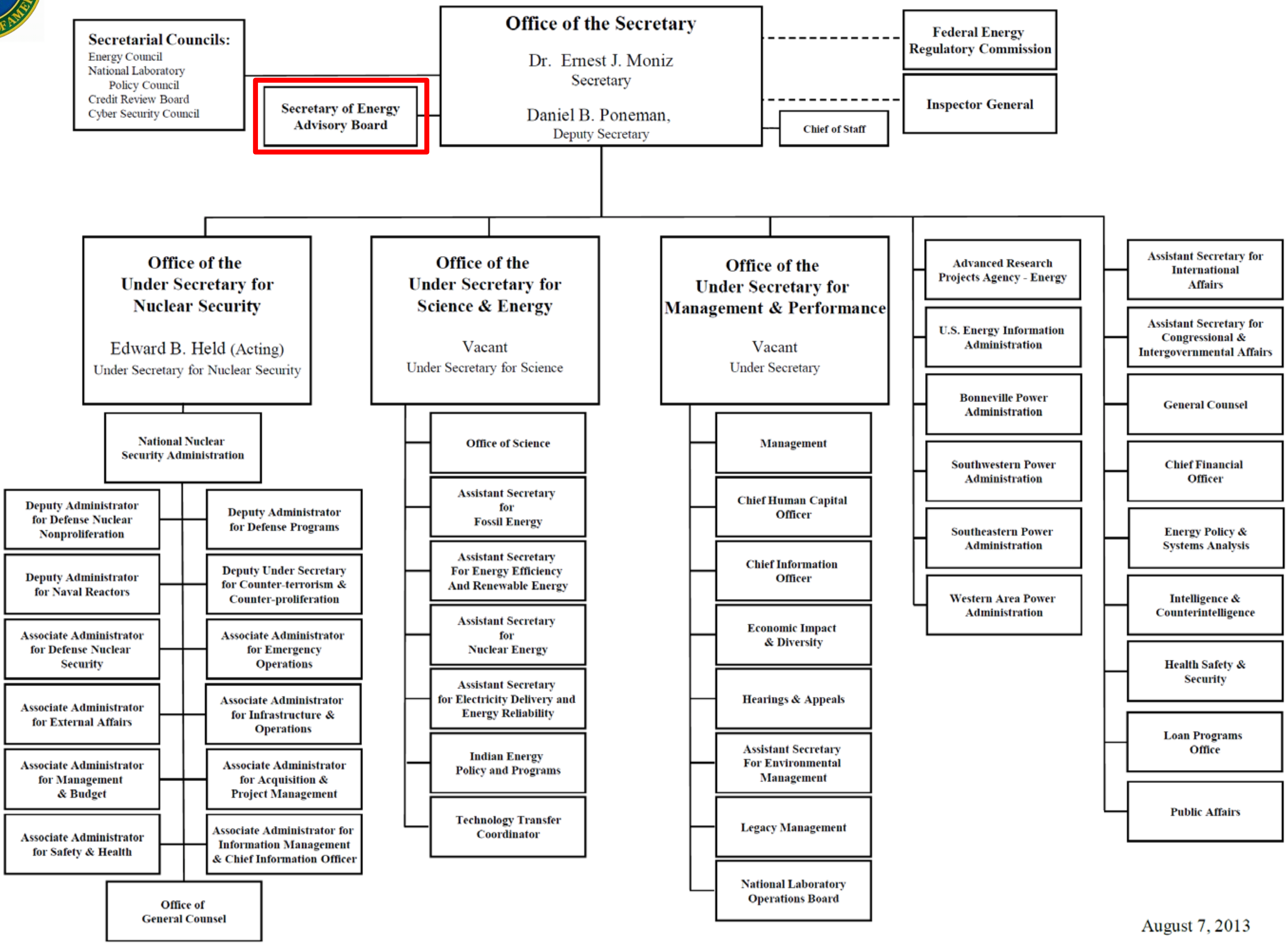

Secretary of Energy Advisory Board*

John Deutch (co-chair) - MIT Chemist and Former Under Secretary of Energy

Persis Drell (co-chair) - Professor of Physics, Stanford University and Former Director, SLAC National Accelerator Laboratory

Frances Beinecke - President, Natural Resources Defense Council

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Deborah Jin - Physicist, National Institute of Standards and Technology and Professor Adjoint for Physics at the University of Colorado, Boulder

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Brent Scowcroft - Retired U.S. Lieutenant General, Former National Security Advisor and President and Founder, Scowcroft Group

Ram Shenoy - Chief Technology Officer, ConocoPhillips

Daniel Yergin - Vice Chairman, IHS and Founder of IHS Cambridge Energy Research Associates

*http://energy.gov/leadership/secretary-energy-advisory-board

SEAB Activities to Date and Planned

- December 3, 2013 – Meeting at LLNL
  - Agreed to establish task force to examine drivers for next-generation, high-performance computing
- March 28, 2014 – Meeting in Washington, DC[†]
  - Reviewed and voted to approve final reports on
    - "Hubs+"
    - FracFocus 2.0
  - Received updates on task-force activities, including
    - Quadrennial Energy Review
    - Nuclear Nonproliferation Study
    - High-Performance Computing
- *June 20, 2014 – Meeting at ANL*

[†]http://www.energy.gov/seab/events/seab-meeting

The Secretary of Energy
Washington, DC 20585

December 20, 2013

MEMORANDUM FOR THE CO-CHAIRS
SECERETARY OF ENERGY ADVISORY BOARD

FROM: ERNEST J. MONIZ

SUBJECT: Establishing a Next Generation High Performance Computing Task Force

I request that you form a Secretary of Energy Advisory Board (SEAB) Task Force composed of SEAB members and independent experts to review the mission and national capabilities related to next generation high performance computing. The Task Force will examine the challenge problems and opportunities that drive the need for next generation high performance computing, as well as the advances and necessary steps to create and execute a successful path that will deliver next generation computational performance. The Task Force report should include recommendations on whether and to what degree the U.S. Government should lead and accelerate the development of next generation high performance computing applications and systems.

Purpose of the Task Force: The SEAB Next Generation High Performance Computing Task Force will examine and report on the following:

- The justification for an exascale computing capability initiative.
    - DOE missions
    - Fundamental research opportunities
    - Broader societal benefits from an open, non-classified exascale program and potential market barriers inhibiting private development of exascale computing
- Related basic research necessary to enable next generation high performance computing (e.g. mathematics, computer science, etc., including quantum and superconducting computing).
- The current state of technology and plans for an exascale program in the Department of Energy and other federal agencies.
- Role of the Department of Energy in leading the development of exascale computing – including its involvement and collaboration with industry, universities and other government agencies on high performance computing.
- Implications of data centric computing for exascale computing.

Designated Federal Official: Amy Bodette, Deputy Director, Office of Secretarial Boards and Councils

Schedule: The Task Force will submit a report by June 2014 and make a presentation at SEAB's June meeting.

SEAB Task Force on Next-Generation High-Performance Computing

- Shirley Ann Jackson, Co-Chair, Rensselaer Polytechnic Institute
- Michael McQuade, Co-Chair, United Technologies Corporation
- Roscoe Giles, Boston University
- Jim Hendler, Rensselaer Polytechnic Institute
- Peter Highnam, IARPA
- Anita Jones, University of Virginia
- John Kelly, IBM
- Steve Koonin, NYU Center for Urban Science and Progress
- Craig Mundie, Microsoft
- Thomas Ohki, Raytheon BBN Technologies
- Dan Reed, University of Iowa
- Ram Shenoy, ConocoPhillips
- Kord Smith, Massachusetts Institute of Technology
- John Tracy, Boeing (Ted Colbert)

Task Force Activities to Date and Planned

- February 11 – Industry Perspectives
  - Industry uses of exascale-class computing
    - Aviation
    - Petroleum
    - “Search” applications
    - Finance Sector
- March 11 – National Security Perspectives
  - Intelligence Community
  - Stockpile Stewardship
- April 1 – Beyond-CMOS Technologies
  - Superconducting
  - Quantum
- May – TBD
- June – deliver final report to Sec. Moniz

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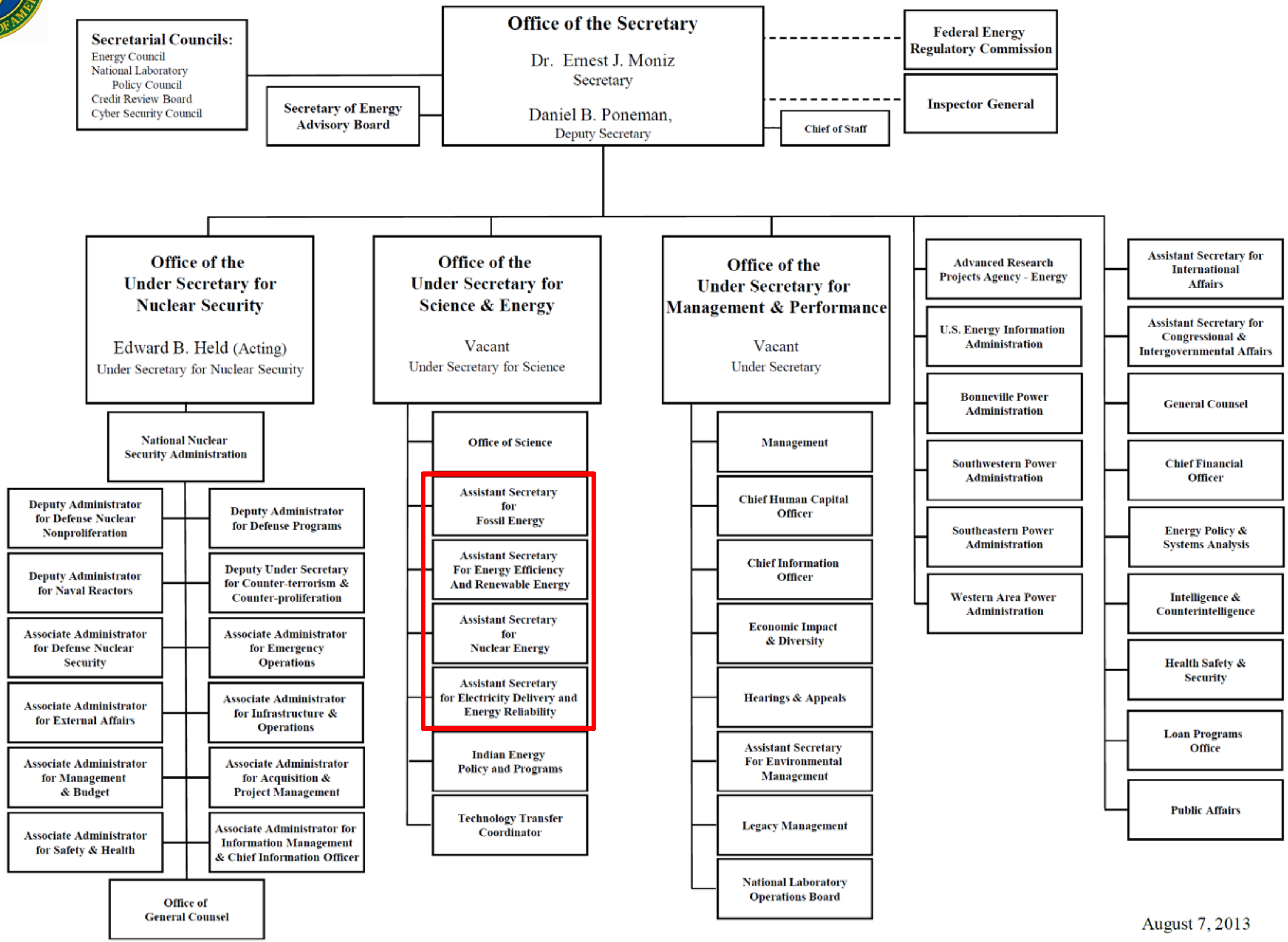


August 7, 2013

DOE Cross-Cutting Initiatives

- Six “Tech Teams” are being organized by the Office of the Under Secretary for Science and Energy
  - Cross-organizational participation
  - Will inform FY 2016 budget formulation
- Applied energy programs
  - Fossil Energy
    - Coal, oil, natural gas
  - Energy Efficiency / Renewable Energy
    - Buildings, Wind, Solar, Transportation, Manufacturing
  - Nuclear Energy
    - Fission technologies, present and future
  - Office of Electricity Delivery and Energy Reliability (the “Grid”)
    - Resiliency, reliability, security

6 Tech Teams Formed Around Key Secretarial Priorities

Advanced Computing

Grid

Manufacturing

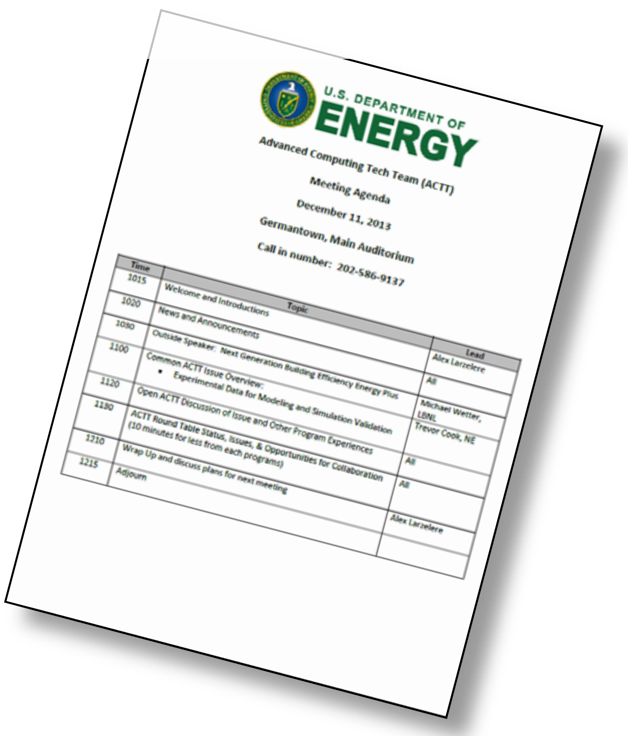
Subsurface

Supercritical CO2

Water-Energy

ACTT History

- Officially Designated a Tech Team in June 2012 by former Secretary Chu
- Meets monthly



U.S. DEPARTMENT OF ENERGY

Advanced Computing Tech Team (ACTT)

Meeting Agenda

December 11, 2013

Germantown, Main Auditorium

Call in number: 202-586-9137

Time	Topic	Lead
1015	Welcome and Introductions	Alex Larzelere
1020	News and Announcements	All
1030	Outside Speaker: Next Generation Building Efficiency Energy Plus	Michael Wetter, LBNL
1100	Common ACTT Issue Overview: • Experimental Data for Modeling and Simulation Validation	Trevor Cook, NE
1120	Open ACTT Discussion of Issue and Other Program Experiences	All
1130	ACTT Round Table Status, Issues, & Opportunities for Collaboration (10 minutes for less from each programs)	All
1210	Wrap Up and discuss plans for next meeting	Alex Larzelere
1215	Adjourn	

- Current Membership:
  - Electrical Delivery (OE)
    - Grid Modeling
  - Energy Efficiency and Renewable Energy (EERE)
    - Wind and Water, Fuel Cell, Vehicle Technologies, Solar
  - Environmental Management (EM)
    - ASCEM (risk management)
  - Fossil Energy (FE)
    - Carbon Capture, NRAP
  - National Nuclear Security Administration (NNSA)
    - Defense Programs ASC, Nonproliferation DNN
  - Nuclear Energy (NE)
    - NEAMS, Energy Innovation Hub
  - Science (SC)
    - ASCR, BER, BES, FES, HEP, NP

ACTT Goals

- Identify impactful, applied-program applications for adaptation to HPC platforms,
- Credibly document the applied-side HPC computing requirements, and
- Identify approaches to accelerate early use of HPC within the applied programs

- Catalog anticipated applied program requirement
- Catalog available advanced computing resources
  - Computational capabilities
  - Applications
  - Supporting technologies and processes (e.g. V & UQ, Demonstration Facilities)
- Identify gaps to inform investment recommendations

ACTT Structure* and Next Steps

- Leadership
  - Co-chaired by an applied program and SC
  - One-year, renewable terms
  - Nominated and approved by DOE management
- Membership
  - Cross-cutting, including NNSA and EM
  - Participatory, self-nominating
  - Interest and subject-matter expertise in advancing use of HPC in DOE programs
- Next steps:
  - Finalize ACTT charter†
  - Conduct initial ACTT Workshop – April 14-15, 2014
    - Leverages on July 31-August 2, 2012 Workshop
    - Explore opportunities to collaborate & share
    - Identify gaps and shortfalls

*Under Development
†In management review

Updates

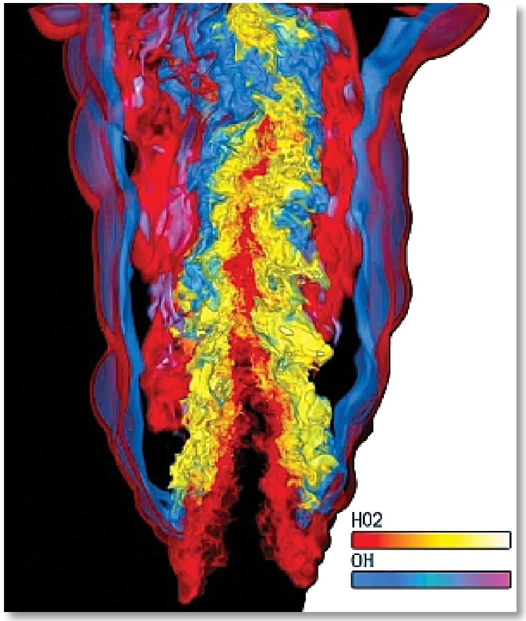
(activities within SC & ASCR)

Program Updates

- **Path toward Exascale**
  - Achieving new, higher levels of concurrency
  - Affordable power consumption
  - Programmability
  - Resiliency
  - Large data
- **ASCR Facilities**
  - Leadership Computing
  - National Energy Research Supercomputing Center (NERSC)
  - High-performance networking
- **Applied math, computer science, SciDAC**
  - Tools, libraries, software to maximally utilize future HPC systems

Mission: Extreme Scale Science
Next Generation of Scientific Innovation

- **In partnership with NNSA**
- **"All-in" approach: hardware, software, applications, large data, underpinning applied math and computer science**
- **DOE's missions push the frontiers of science and technology:**
  - Discovery science
  - Mission-focused basic science in energy
  - Provide state-of-the-art scientific tools
  - Plan, implement, and operate user facilities
- **The next generation of advancements will require Extreme Scale Computing**
  - 1,000X capabilities of today's computers with a similar physical size and power footprint
- **Extreme Scale Computing, cannot be achieved by a "business-as-usual," evolutionary approach**



Path Toward Exascale in FY 2015

Mathematical, Computational, and Computer Sciences Research

- **Uncertainty Quantification:** Continues support for awards made in 2013 on "UQ methods for Extreme-Scale Science" These efforts will improve the fidelity and predictability of DOE simulations.
- **Extreme scale Advanced Architectures:** Supports new research addressing *in situ* methods, workflows, and proxy applications for data management, processing, analysis and visualization; continues support for research into advanced architectures, software environments and operating systems
- **Co-Design:** Continues support for Co-Design activities, including data-intensive science partnerships started in FY 2014

High Performance Computing and Network Facilities

- **Platform R&D and Critical Technologies:** Initiates conceptual design studies for prototypical exascale systems from application workflow to hardware structure and system software; continues support for Fast Forward investments in critical technologies and Design Forward investments in system-level engineering efforts with high performance computer vendors

Research & Evaluation Prototypes (+$20,150K)

- **FastForward:** In FY 2012, Research and Evaluation Prototypes activity worked with NNSA to award $95M (total, including cost sharing, over two years) for innovative R&D on critical technologies – memory, processors and storage – needed to deliver next generation capabilities within an affordable energy footprint.
  - **Funded Projects:**
    - AMD: processors and memory for extreme systems;
    - IBM :   memory for extreme systems;
    - Intel Federal: energy efficient processors and memory architectures;
    - Nvidia: processor architecture for exascale computing at low power; and
    - Whamcloud: storage and I/O (input/output) – *subsequently bought by Intel*.
- The FY 2015 increase takes FastForward research to the next level:
  - Lab/vendor partnerships (+$12,216K)
    - develop prototypes of the most promising mid-term technologies from the Fast Forward program for further testing.
  - Nonrecurring engineering (+$7,934K)
    - Incorporate near-term technologies from Fast Forward into planned facility upgrades at NERSC, ALCF and OLCF.

Development of Next-Generation Applications

(funded within domain-science programs)

BES +$24.2M **Computational materials sciences** to develop research codes for design of functional materials.

BER +$29.0M **Climate model development and validation** – combine advanced software code development and numerical methods with new ARM data to design an Earth system model with sub-10km resolution.

Leadership and Production Computing Facilities

Titan:

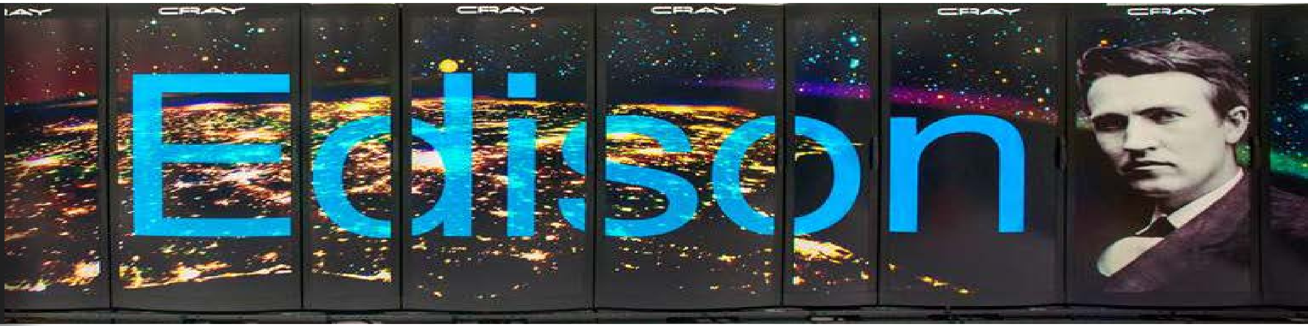
- Peak performance of 27.1 Petaflops
- 18,688 Hybrid Compute Nodes
- 8.9 MW peak power

Mira:

- Peak performance of 10 Petaflops
- 49,152 Compute Nodes
- 4.8 MW peak power

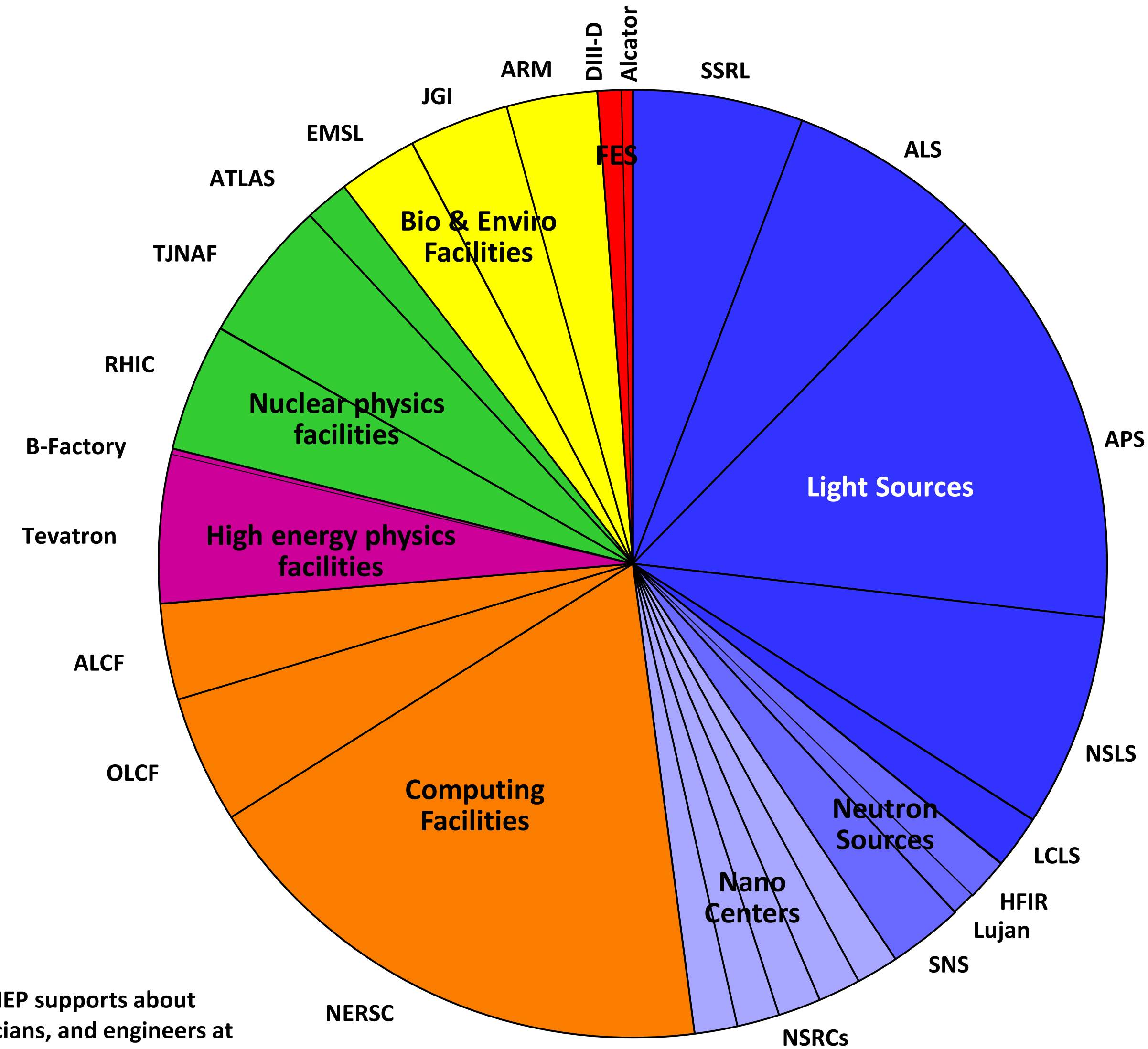
Edison XC30:

- Peak performance 2.4PF
- 5,576 Compute Nodes
- 2.1 MW peak power



Distribution of Users at the ~30 SC Facilities 2013

Nearly ¾ of users do their work at ASCR or BES facilities

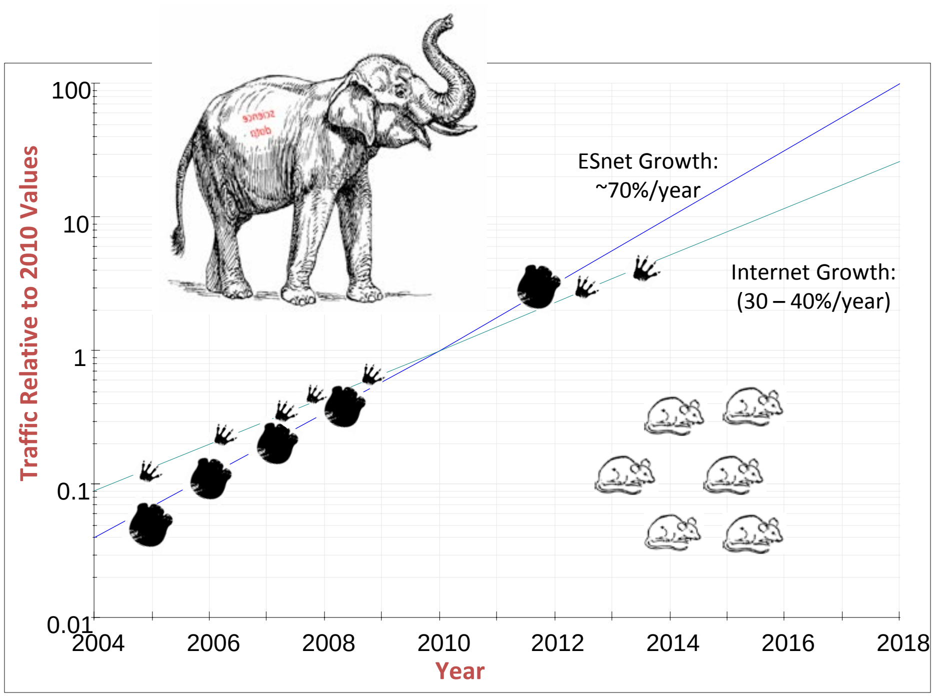


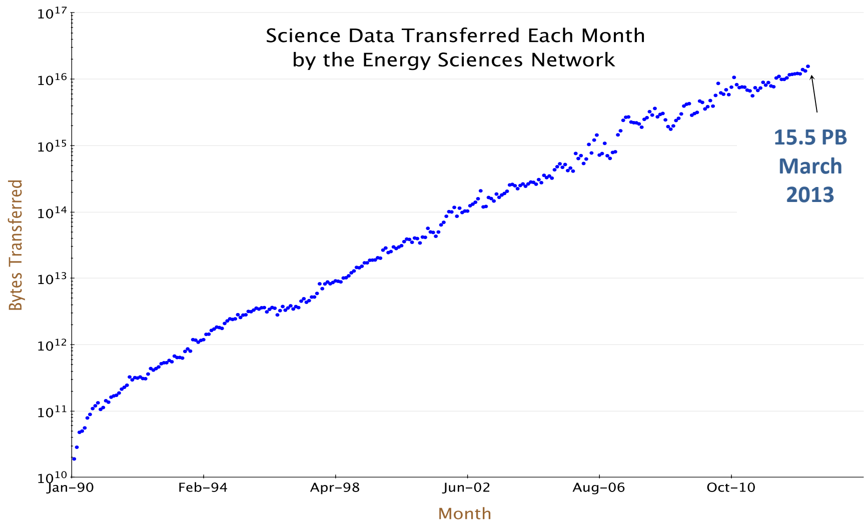
Does not include LHC; HEP supports about 1,700 scientists, technicians, and engineers at the LHC.

ESNET: World's First Continental 100 Gbs Production Network

Network Specifications:

- 16 Alcatel Lucent routers, plus new Ciena optical platform
- Network can grow to 88 independent 100G channels
- Deploying 100G production connections at ANL, BNL, FNAL, LBNL, LLNL, NERSC, ORNL in next 6 months
- Improved fiber and optical diversity
- >99.99% availability to Labs in CY2012





ESnet grows twice as fast as the commercial Internet, due largely to *elephant flows* and data intensive science.

FY 2015 ASCR Facility Investments (in $K)

- NERSC (High Performance Production Computing) (+3,395):
  - Operate optimally (over 90% scheduled availability)
  - Move to the Computational Research and Theory Building back on the LBNL campus
  - Initiate a post-doctoral training program for high-end computational science and engineering
- LCFs (+13,320 ALCF; +11,300 OLCF)
  - Operate optimally (over 90% scheduled availability)
  - Prepare for planned 75-200 petaflop upgrades in the 2017-2018 timeframe
  - Initiate a post-doctoral training program for high-end computational science and engineering
- High Performance Network Facilities and Testbeds (+2,300)
  - Operate optimally (99.99% reliability)
  - Coordinate with other agencies to ensure the availability of next generation of optical networking from domestic sources
  - Expansion of 100 Gbs network to support interim traffic growth

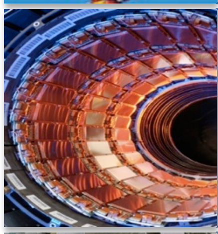
Office of Science and "Big Data"

- SC is viewed by many not to be a player in "big data"
- However, examples within SC abound:
  - Data from large-scale experiments (HEP, BES); medium-scale experiments (BER)
  - Observational data (BER/Climate, BER/Environment, HEP)
  - Simulation results (BER/Climate, BES, HEP, NP, FES)
- SC has significant infrastructure devoted to data
  - ASCR: NERSC and the Leadership Computing Facilities
  - HEP: data architecture devoted to LHC
- Big data and big computing go hand-in-hand – cannot have one without the other
- A confluence of large experimental facilities and high-end computing is beginning to occur
  - ALS, APS, LCLS, SNS
- New approaches for partnering may be needed
- Note: there are significant efforts/interest across the US Government (NIST, NSF, OSTP, OMB)

Mission: Extreme-Scale Science Data Explosion

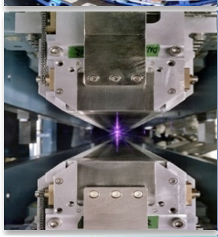
Genomics

Data Volume increases to 10 PB in FY21



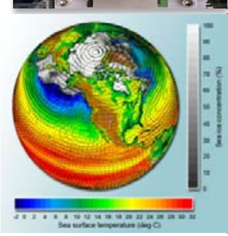
High Energy Physics (Large Hadron Collider)

15 PB of data/year



Light Sources

Approximately 300 TB/day



Climate

Data expected to be hundreds of 100 EB

Driven by exponential technology advances

Data sources

- Scientific Instruments
- Scientific Computing Facilities
- Simulation Results
- Observational data

Big Data and Big Compute

- Analyzing Big Data requires processing (e.g., search, transform, analyze, …)
- Extreme scale computing will enable timely and more complex processing of increasingly large Big Data sets

Data drivers from DOE Scientific User Facilities†

	2013 Current data rate*	2015 Projected need	2018 Projected need
HEP Cosmic Frontier example – Large Synoptic Survey Telescope	~0.2 GB/s	~0.5 GB/s	~1-10 GB/s
HEP Energy Frontier Example – Atlas LHC	1 GB/s*	2 GB/s*	4 GB/s*
HEP Intensity Frontier Example – Belle II	1 GB/s	2 GB/s	20 GB/s
BER Climate	100 GB/s	1000 GB/s	1000 GB /s
BER EMSL – one instrument example - TEM	100 – 1000 images (2Kx2K)/ per day	1000 Images/s = 2GB/s	1,000,000 Images/s = 2 TB/s
BER JGI example - Illumina HiSeq	18 MB/s	72 MB/s	600 MB/s
BES Advanced Photon Source example – 2-BM Beamline	1 GB/s/beamline		10 GB/s
BES Nano Science example – X-Ray Spectroscopy		100 MB x 100 excited atoms x 100 snapshots = 1 TB per point (P,T)	
BES Neutron Facilities	~0.05GB/s	~0.10 GB/s	~0.30GB/s

* Data Rate after 99% reduction in hardware data acquisition system

† http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/ASKD_Report_V1_0.pdf

ASCR Research Investments in “Big Data”

- Applied Math (+$2,655):
  - Development of mathematical algorithms that accommodate the spatial and temporal variation in data and account for the characteristics of sensors as needed and adaptively reduce data
  - Development of new compression techniques
- Computer Science (+3,687)
  - Develop new paradigm for generating and executing dynamic workflows that include the development of new workflow engines and languages that are semantically rich and allow interoperability or interchangeably in many environments
  - Development of scalable and interactive visualization methods for ensembles, multivariate and multiscale data
  - Define components and associated Application Programing Interfaces for storing , annotating and accessing scientific data; support development of standards
- Next Generation Networking for Science (+$3,569)
  - Develop new methods for scheduling data movement over the WAN that includes understanding replication policies, data architectures and subset access mechanisms
  - Create new methods for rapid and scalable collaborative analysis and interpretation
  - Construct a cyber framework that supports complex real-time analysis and knowledge navigation, integration and creation processes.

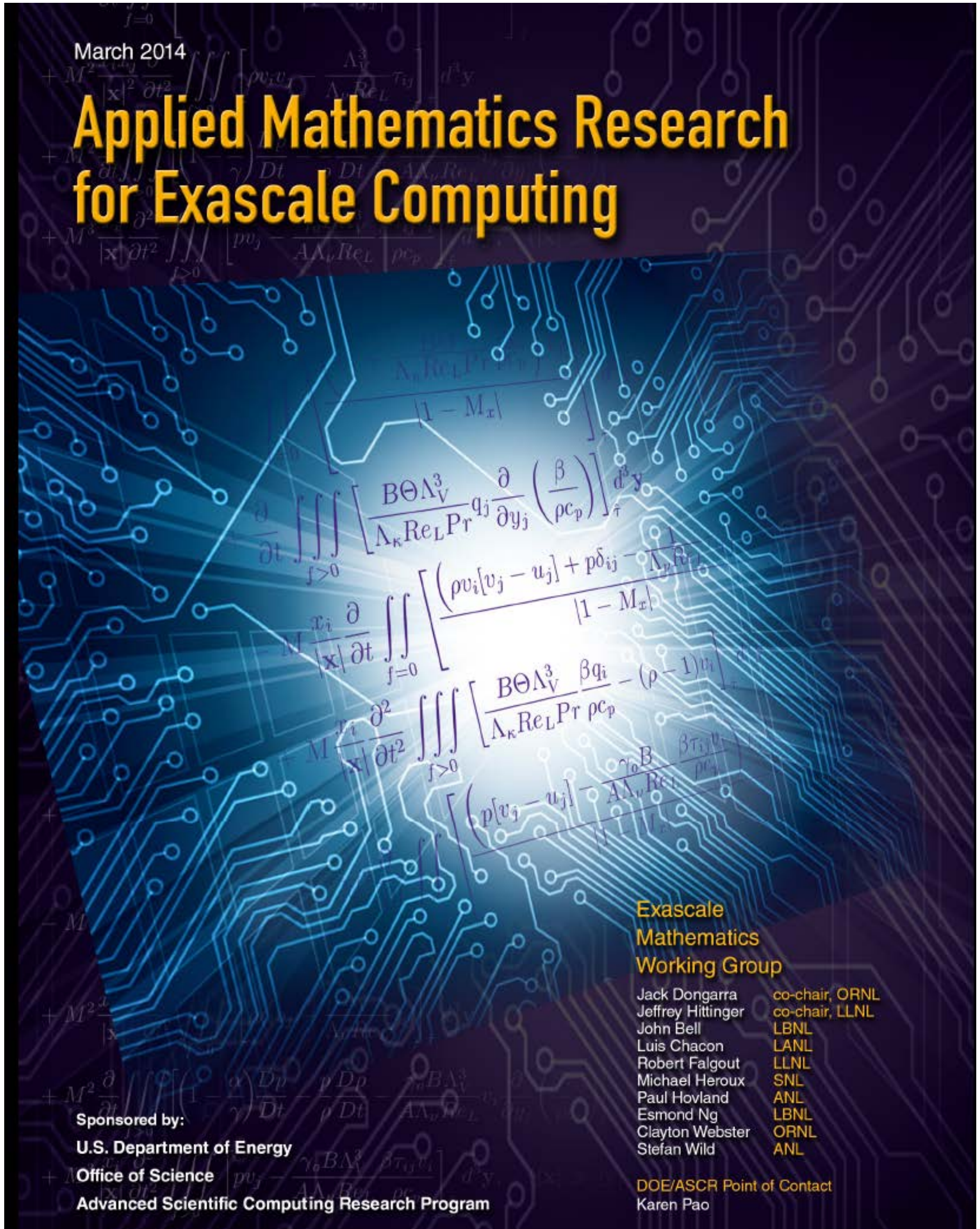
Next Steps

In FY 2014:

- Develop concepts for SC-wide data architecture
- Identify a small number of large-data data demonstrations that are relevant to SC domain programs
- Identify common software tools and stacks needed at both the domain level and system wide
- Identify needed computer science and applied mathematics to advance the field of large-data exploitation for scientific applications.

In FY 2015:

- Develop initial baseline plan for system-wide architecture, based on conceptual planning and demonstrations conducted in FY 2014 and begin implementation of initial architecture
- Expand 2-3 of the FY 2014 demonstration projects into pilot studies to validate selected, domain-specific data applications
- Initiate development of system-wide middleware tools and new algorithms for new detectors and in situ analysis
- Begin exploration of a few pilots and start on tools to support end to end solutions such as middleware tools



https://collab.mcs.anl.gov/display/examath/Exascale+Mathematics+Home

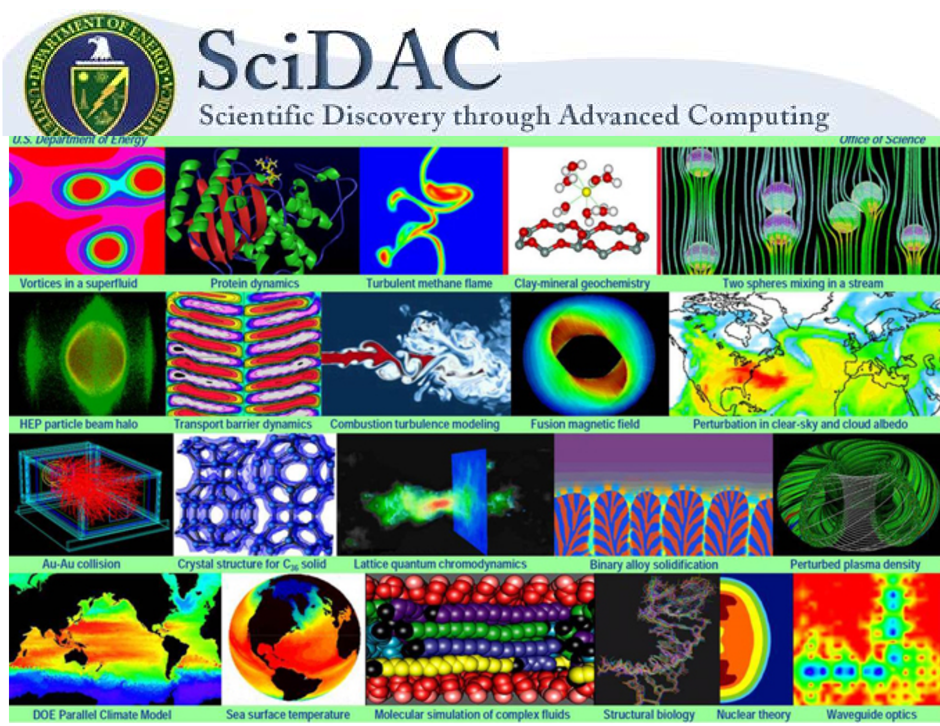
Applied Mathematics Research for Exascale Computing

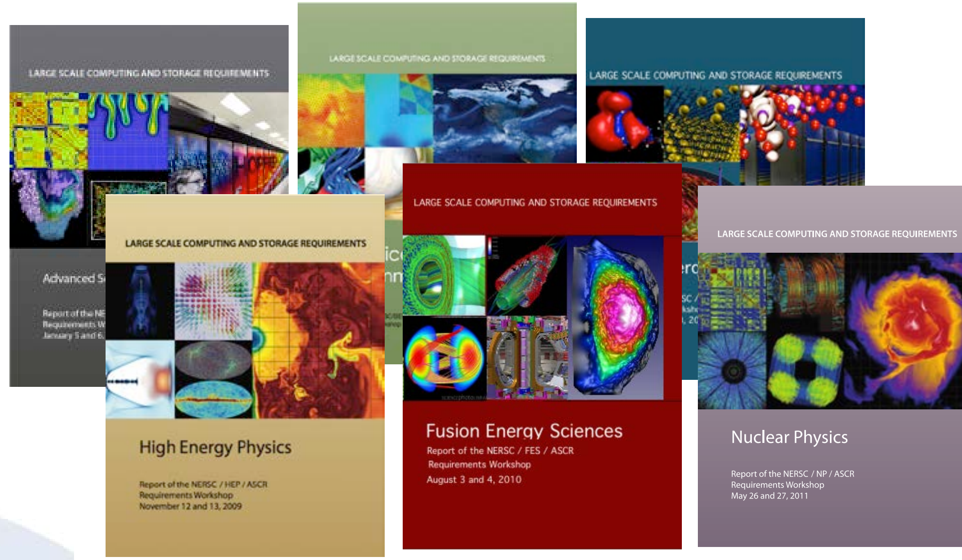
“Concisely, the DOE Advanced Scientic Computing Research Program needs to take action to build a more explicit research program in applied mathematics for exascale computing. The necessary actions are summarized in five key recommendations:

1. DOE ASCR should proceed expeditiously and with high priority with an exascale mathematics initiative so that DOE continues to lead in using extreme-scale computing to meet important national needs.
2. A significant new investment in research and development of new models, discretizations, and algorithms implemented in new science application codes is required in order to fully leverage the significant advances in computational capability that will be available at the exascale. Many existing algorithms and implementations that have relied on steady clock speed improvements cannot exploit the performance trends of future systems.
3. Not all problems require exascale computation, and yet these problems will continue to require applied mathematics research. Thus, a balance is needed in the DOE Applied Mathematics Research portfolio that provides sufficient resources to realize the potential of exascale simulation while preserving a healthy base research program.
4. An intensive co-design effort is essential for success, where computer scientists, applied mathematicians, and application scientists work closely together to produce a computational science discovery environment able to exploit the computational resources that will be available at the exascale.
5. DOE ASCR must make investments to increase the pool of computational scientists and mathematicians trained in both applied mathematics and high-performance computing.”

ASCR Partnerships Across the Office of Science

- SciDAC
  - Partnerships facilitate transfer of ASCR research results into SC applications
  - Third generation, 18 partnerships across SC and 4 SciDAC Institutes





Requirements gathering for facility upgrades

- NERSC, ALCF, OLCF
- ESnet

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/

END