U.S. DEPARTMENT OF ENERGY

DOE Office of Advanced Scientific Computing Research

Presented to the
Advanced Scientific Computing Advisory Committee

by

Steve Binkley
Associate Director

November 21, 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%

FY15 ASCR Appropriations: HEWD vs. SEWD

HEWD Committee Report

ADVANCED SCIENTIFIC COMPUTING RESEARCH

The Advanced Scientific Computing Research program develops and hosts some of the world's fastest computing and network capabilities to enable science and energy modeling, simulation, and research. The Committee recommends $541,000,000 for Advanced Scientific Computing Research, $62,407,000 above fiscal year 2014 and the same as the budget request.

Exascale Computing.—The Committee continues to support the exascale initiative, which seeks to develop the next generation of computing systems three orders of magnitude faster than today's fastest systems. This decade-long effort is critical to enabling basic and energy-focused science research not previously possible and to maintaining the nation's global leadership in computing technologies. The recommendation includes the requested level of $91,000,000.

High Performance Computing and Network Facilities.—In addition to the long-term exascale intiative, the Committee supports continued upgrade and operation of the Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories and of the High Performance Production Computing capabilities at Lawrence Berkeley National Laboratory. These systems' capabilities are a critical component of science and industrial research and development across the nation, and they should be maintained as world leading facilities. The recommendation includes the requested levels of $80,320,000 for the Argonne Leadership Computing Facility; $104,317,000 for the Oak Ridge Leadership Computing Facility; and $69,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory.

All other activities within the Advanced Scientific Computing Research program are funded at the requested level.

SEWD Committee Report

EXASCALE INITIATIVE

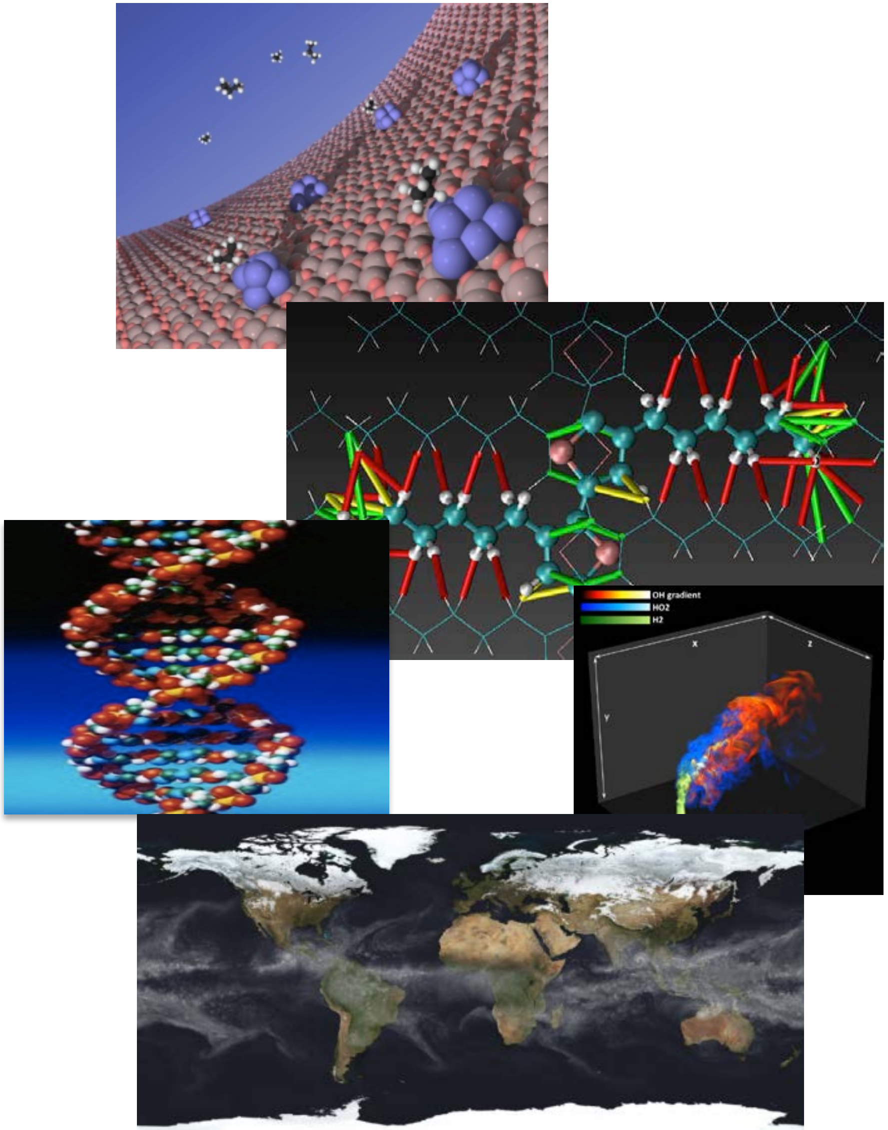
The Committee recommends $151,000,000, which includes $91,000,000 for the Office of Science and $60,000,000 for the National Nuclear Security Administration [NNSA], to support the Department's initiative to deploy the first exascale system by 2022. The Committee believes the United States must remain the world leader in high performance computing. Virtually every sector of U.S. society has become dependent on the continued growth in computing performance to advance science and technology, drive industrial productivity, and accelerate innovation. The Committee encourages the Department to continue making investments in exascale systems one of its highest priorities.

ADVANCED SCIENTIFIC COMPUTING RESEARCH

The Committee recommends $557,000,000, an increase of $16,000,000 above the request, for Advanced Scientific Computing Research. The Committee believes its recommendation would allow the Department to develop and maintain world-class computing and network facilities for science and deliver the necessary research in applied mathematics, computer science, and advanced networking to support the Department's missions. Within these funds, the Committee recommends $91,000,000 as requested for the exascale initiative to spur U.S. innovation and increase the country's ability to address critical national challenges. The Committee supports the Department's plan to deploy by 2022 the first exascale system that is energy efficient and can help solve the most pressing energy, national security, and environmental challenges.

The Committee also recommends $104,317,000 for the Oak Ridge Leadership Computing Facility, $80,320,000 for the Argonne Leadership Computing Facility, and $85,000,000 for the National Energy Research Scientific Computing Center [NERSC] facility at Lawrence Berkeley National Laboratory. The Committee recommends additional funding for NERSC to avoid a loss of 1 billion hours, or 33 percent, of computing time available to scientists in 2015. The additional funding is provided to expand the NERSC–7 systems to make up for lost capability when NERSC–6 is decommissioned and make power and cooling upgrades to the new Computational Research and Theory Facility.

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

Updates

- **FY 2015 Budget**
- **CSGF**
- **Appointees**
- **ASCR Personnel Changes**
  - Christine Chalk: Oak Ridge Leadership Computing
  - Robinson Pino: HPC Science and Applications*
  - Carolyn Lauzon: ALCC Program Manager*
  - Ravi Kapoor (departed)

*new hire

Report of the Task Force on High Performance Computing of the Secretary of Energy Advisory Board

August 10, 2014

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.

Task Force and Study Participants

SEAB Members

Shirley Ann Jackson, Co-Chair, Rensselaer Polytechnic Institute
Michael McQuade, Co-Chair, United Technologies Corporation
Ram Shenoy, ConocoPhillips
Steve Koonin, NYU Center for Urban Science and Progress

External Participants

Roscoe Giles, Boston University
Jim Hendler, Rensselaer Polytechnic Institute
Peter Highnam, IARPA
Anita Jones, University of Virginia
John Kelly, IBM
Craig Mundie, Microsoft
Thomas Ohki, Raytheon BBN Technologies
Dan Reed, University of Iowa
Kord Smith, Massachusetts Institute of Technology
John Tracy, Boeing (Ted Colbert)

Key Findings

1. Investable needs exist for an exascale class machine.
   a. The historical NNSA mission (simulation for stewardship), multiple industrial applications (e.g., oil and gas exploration and production, aerospace engineering and medicinal chemistry (pharmaceuticals, protein structure, etc.)) and basic science all have applications that demonstrate real need and real deliverables from a significant performance increase in classical high performance computing at several orders of magnitude beyond the tens of petaflop performance delivered by today's leadership machines.
2. Significant, but projectable technology development can enable one last "current" generation machine.
   a. Optimization of current CMOS, highly parallel processing within the remaining limits of Moore's law and Dennard scaling likely provides one last "generation" of conventional architecture at the 1-10 exascale performance level, within acceptable power budgets. Significant, but projectable technology and engineering developments are needed to reach this performance level.
3. "Classical" high end simulation machines are already significantly impacted by many of the data volume and architecture issues.
   a. The performance of many complex simulations is less dominated by the performance of floating point operations, than by memory and integer operations.
   b. As the data sets used for classic high performance simulation computation become increasingly large, increasingly non-localized and increasingly multi-dimensional, there is significant overlap in memory and data flow science and technology development needed for classic high performance computing and for data centric computing.
4. Data-centric at the exascale is already important for DOE missions.
   a. There is an evolution already underway in the DOE computing environment to one that supports more memory- and integer-operation dominated simulation for the NNSA security mission.
   b. Applications of data centric computing for DOE, for other parts of the U. S. Government, and for the private sector, are rapidly scaling to and beyond levels of performance that are comparable to the those needed for classic high performance floating point computation.

Key Findings, continued

5. Common challenges and under-girding technologies span computational needs.
    a. As the complexity of data-centric problems increases, the associated calculations face the same challenges of data movement, power consumption, memory capacity, interconnection bandwidth, and scaling as does simulation-based computations.
6. The factors that drive DOE's historical role in leadership computing still exist and will continue.
    a. The DOE National Labs are an important and unique resource for the development of next generation high performance computing and beyond.
    b. The DOE partnering mechanisms with industry and academia have proven effective for the last several generations of leadership computing programs.
    c. Because of its historical and current expertise in leading the development of next generation high performance computing, the DOE has a unique and important role to play in the National Strategic Computing Initiative.
7. A broad and healthy ecosystem is critical to the development of exascale and beyond systems.
    a. Progress in leading-edge computational systems relies critically on the health of the research environment in underlying mathematics, computer science, software engineering, communications, materials and devices, and application/algorithm development.
8. It is timely to invest in science, technology and human investments for "Beyond Next".
    a. A number of longer term technologies will be important to "beyond next" generation high performance computing (superconducting, quantum computing, biological computation), but are not mature enough to impact the next leading edge capability investments at DOE.

Summary of Recommendations

1. **DOE, through a program jointly established and managed by the NNSA and the Office of Science, should lead the program and investment to deliver the next class of leading edge machines by the middle of the next decade. These machines should be developed through a co-design process that balances classical computational speed and data-centric memory and communications architectures to deliver performance at the 1-10 exaflop level, with addressable memory in the exabyte range.**
2. **This program should be executed using the partnering mechanism with industry and academia that have proven effective for the last several generations of leadership computing programs. The approximate incremental investment required is $3B over 10 years.**
3. **DOE should lead, within the framework of the National Strategic Computing Initiative (NSCI), a co-design process that jointly matures the technology base for complex modeling and simulation and data centric computing. This should be part of a jointly tasked effort among the agencies with the biggest stake in a balanced ecosystem.**
4. **DOE should lead a cross-agency U. S. Government (USG) investment in "over-the-horizon" future high performance computing technology.**
5. **DOE should lead the USG efforts to invest in maintaining the health of the underlying balanced ecosystem in mathematics, computer science, new algorithm development, physics, chemistry, etc.**

We note that the combined DOE investment in maintaining a healthy ecosystem and pursuing over-the-horizon technology identification and maturation is in the range of $100-150M per year.

National Strategic Computing Initiative

National Strategic Computing Initiative – NSCI

NSCI Mission: To maintain US strategic advantage in HPC for security, discovery, and the economy in the near term and beyond Moore's Law

- OSTP/NSTC task force, established November 2013
  - Led by Patricia Falcone, Associate Director for National Security
  - Charged to define USG approach to HPC for next decade, in time to inform FY 2016 budget
- Membership comprises all federal agencies with equity in HPC
  - Executive Office of the President (OSTP, OMB)
  - DOE (SC, NNSA, Energy, Labs)
  - Intelligence Community (IARPA, CIA, NSA)
  - DoD (HPCMod)
  - DOC (NIST, NOAA)
  - NASA
  - NIH
  - NSF

NSCI Intent

Definitions and scope:

- HPC = most advanced, capable computing technology available in a given era
- Multiple styles of computing and all necessary infrastructure
- Scope includes everything necessary for a fully integrated capability
  - Theory and practice, software and hardware

Approach:

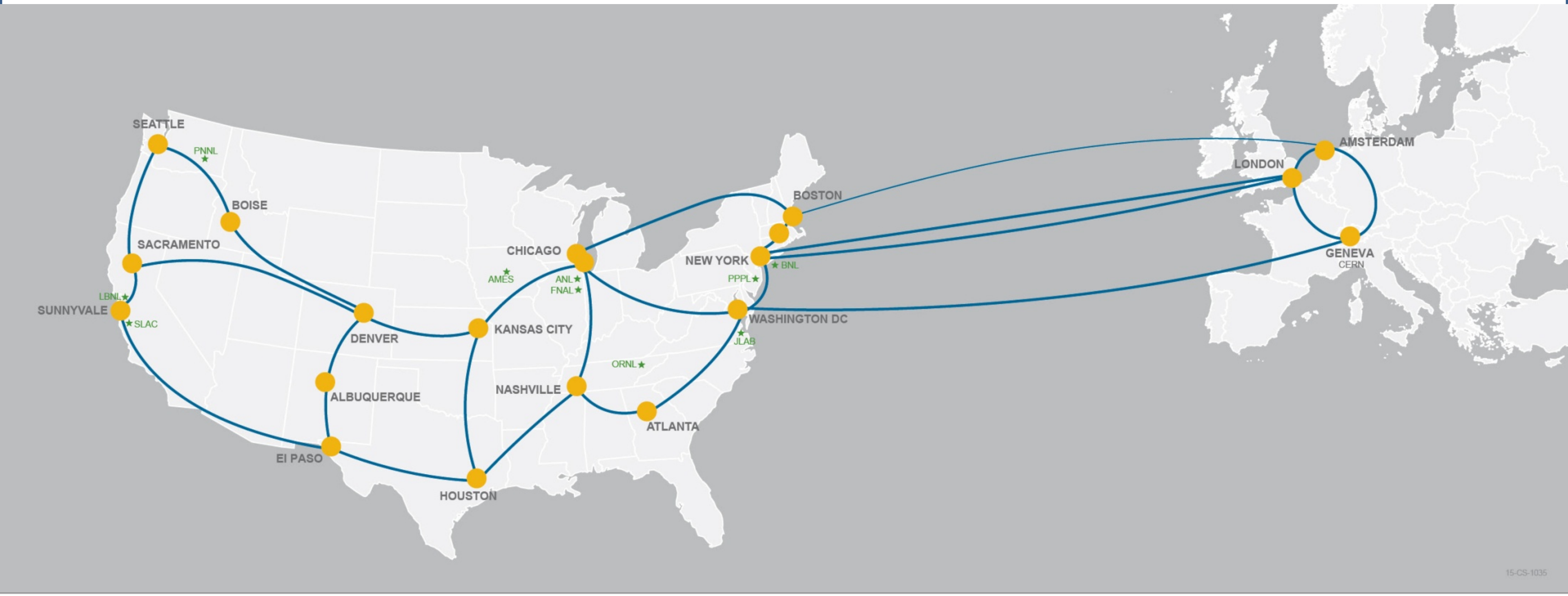
- "Whole of government" approach
  - Leverage beyond individual programs
  - Link and lift efforts across USG
- Public/private partnership with industry, academia, labs
- Long time horizon – a decade or more

Program Updates

- **Path toward Exascale**

- **ASCR Facilities**
  - Leadership Computing – Update on CORAL acquisition
  - National Energy Research Supercomputing Center (NERSC) – Update on Cori acquisition
  - ESnet extension to Europe

- **Applied math, computer science, SciDAC**
  - Next-Generation Networking



ESnet

ENERGY SCIENCES NETWORK

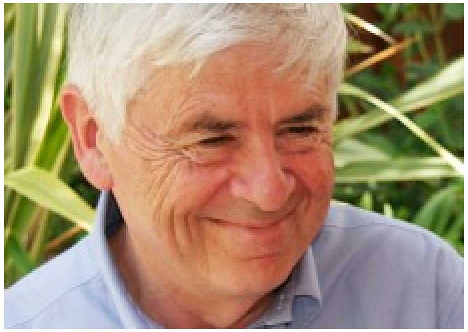
★ Department of Energy Office of Science National Labs

Ames	Ames Laboratory (Ames, IA)
ANL	Argonne National Laboratory (Argonne, IL)
BNL	Brookhaven National Laboratory (Upton, NY)
FNAL	Fermi National Accelerator Laboratory (Batavia, IL)
JLAB	Thomas Jefferson National Accelerator Facility (Newport News, VA)
LBNL	Lawrence Berkeley National Laboratory (Berkeley, CA)
ORNL	Oak Ridge National Laboratory (Oak Ridge, TN)
PNNL	Pacific Northwest National Laboratory (Richland, WA)
PPPL	Princeton Plasma Physics Laboratory (Princeton, NJ)
SLAC	SLAC National Accelerator Laboratory (Menlo Park, CA)

ASCR Researchers Recognized

Chorin wins National Medal of Science

Alexandre Chorin, a mathematician with Berkeley Lab's Computational Research Division and a University Professor of mathematics at UC Berkeley, was named as a recipient of the National Medal of Science, the nation's highest honor for achievement and leadership in advancing the fields of science and technology.



Alexandre Chorin

In a career that spans nearly 50 years, Chorin is internationally recognized for signature contributions to turbulence modeling, as well as other critical areas in applied mathematics and fluid and statistical mechanics.

Chorin has applied his methods to understanding water flow in oceans and lakes, flow in turbines and engines, combustion, and blood flow in the heart and veins.

ASCR Researchers Recognized

PETSc team receives the 2015 SIAM/ACM Prize in Computational Science and Engineering

The prize "is awarded by the Society for Industrial and Applied Mathematics (SIAM) and the Association for Computing Machinery (ACM) in the area of computational science in recognition of outstanding contributions to the development and use of mathematical and computational tools and methods for the solution of science and engineering."

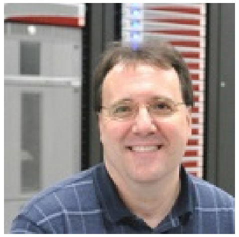
Satish Balay

Jed Brown

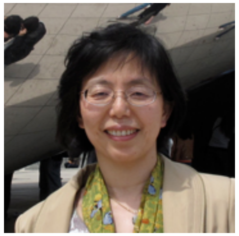
Bill Gropp

Matt Knepley

Lois Curman McInnes



Barry Smith



Hong Zhang

PETSc, Portable, Extensible Toolkit for Scientific Computation, is a numerical software package for the scalable solution of scientific applications modeled by partial differential equations.

PETSc "has transformed the way large-scale software libraries are developed, supported, and used within the CS&E community," according to the SIAM/ACM press release, and its impact "has been felt worldwide."

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/

OSTI Charge

- **OSTI's mission is to maintain, within the Department, publicly available collections of scientific and technical information resulting from research, development, demonstration, and commercial applications activities supported by the Department.**
- **Background:**
  - OSTI was established in 1947 to fulfill the agency's responsibilities associated with the collection, preservation, and dissemination of scientific and technical information from DOE R&D activities, both classified and unclassified.
  - This responsibility was codified in the enabling legislation of DOE and its predecessor agencies and, more recently, was defined as a specific OSTI responsibility in the Energy Policy Act of 2005.

OSTI Charge, continued

- With today's requirements for broad sharing of digital data and open access of publications, the "collection, preservation, and dissemination of scientific and technical information from DOE R&D activities" assumes a complexity impossible to have imagined when OSTI was formed nearly 70 years ago.
- External, independent advice is needed as OSTI transitions its products and services to methods appropriate to the new era of information gathering and sharing.

OSTI Charge, continued

As its first activity, the ASCAC-STI subcommittee is asked to examine the following and provide me with a report by the late-spring or summer 2015 meeting of ASCAC:

a. **Are current OSTI products and services best in class and are they the most critical for the OSTI mission given the present constrained budget environment?**
b. **Do OSTI products and services fulfill customer needs now?**
c. **Are the OSTI products and services positioned to evolve to fulfill customer needs in the future? Has the OSTI strategic plan appropriately addressed the rapid evolution of technologies, research product types, and ways in which research results are communicated and shared?**
d. **What is the national and international standing of OSTI with respect to similar organizations whether at other U.S. Federal Agencies, DOE Laboratories, or universities? In what areas must OSTI be a clear leader to fulfill its mandated responsibilities to the DOE?**

List of Questions

- **User "experience"**
  - Is the set of services appropriate? Adequate? Relevant?
  - Ability for users to find relevant OSTI information
- **Ability to anticipate and intersect future STI needs**
  - Rapidly changing area
  - Evolving use cases for data: types of data, modes of sharing
- **National/international standing**
  - Best in class?
  - In what areas does OSTI need to excel?
- **Other questions:**
  - Extent to which DOE/NNSA laboratories provide reports
  - Robustness of OSTI operation (Reliability, Redundancy, Security)
  - Classified holdings

END