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)

<table>
<thead>
<tr>
<th>FY 2013 Current (prior to SBIR/STTR)</th>
<th>FY 2013 Current Appropriation</th>
<th>FY 2014 Enacted Appropriation</th>
<th>FY 2015 President’s Request</th>
<th>FY15 President’s Request vs. FY14 Enacted Appropriation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Advanced Scientific Computing Research</td>
<td>417,778</td>
<td>405,000</td>
<td>478,093</td>
<td>541,000</td>
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<tr>
<td>Basic Energy Sciences</td>
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<td><strong>Subtotal, Office of Science</strong></td>
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<td><strong>4,504,987</strong></td>
<td><strong>5,066,372</strong></td>
<td><strong>5,111,155</strong></td>
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<td>Small Business Innovation Research/Technology Transfer</td>
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<td>Use of Prior Year Balances</td>
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<tr>
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<td><strong>4,681,195</strong></td>
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**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 initiative, 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.

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**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.
• Investment Priorities

– Conduct research and development, and design efforts in hardware software, and mathematical technologies that will produce exascale systems in 2022.

– 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.

– Acquire and operate more capable computing systems, from multi-petaflop through exascale computing systems that incorporate technologies emerging from research investments.
## ASCR Budget Overview

### Advanced Scientific Computing Research

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<thead>
<tr>
<th>Category</th>
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<tr>
<td>Applied Mathematics</td>
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<td>Computational Partnerships (SciDAC)</td>
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<td>Next Generation Networking for Science</td>
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<td>SBIR/STTR</td>
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<td>High Performance Production Computing (NERSC)</td>
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<td>Leadership Computing Facilities</td>
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<td>Research and Evaluation Prototypes</td>
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<td>SBIR/STTR</td>
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<tr>
<td><strong>Total, High Performance Computing and Network Facilities</strong></td>
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<td><strong>305,646</strong></td>
<td><strong>358,125</strong></td>
<td><strong>+52,479</strong></td>
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• **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
MEMORANDUM FOR THE CO-CHAIRS
SECRETARY 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.
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.
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
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
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
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.

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.
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.”

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.”*
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’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.
• 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.
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