DOE Office of Advanced Scientific Computing Research

Presented to the
Advanced Scientific Computing Advisory Committee

by

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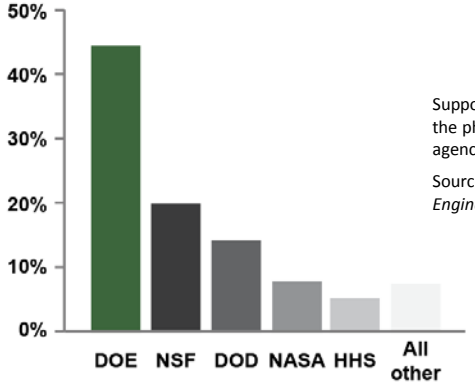
Office of Science
By the numbers

Shown is a portion of SLAC's two-mile-long linear accelerator (or linac), which provides the electron beam for the new Linac Coherent Light Source (LCLS) – the world's first hard x-ray, free-electron laser. For nearly 50 years, SLAC's linac had produced high-energy electrons for physics experiments. Now researchers use the very intense X-ray pulses (more than a billion times brighter than the most powerful existing sources) much like a high-speed camera to take stop-motion pictures of atoms and molecules in motion, examining fundamental processes on femtosecond timescales.

SC delivers scientific discoveries and tools to transform our understanding of nature and advance the energy, economic, and national security of the U.S.

Research

- Support for 47% of the U.S. Federal support of basic research in the physical sciences;
- ~22,000 Ph.D. scientists, grad students, engineers, and support staff at >300 institutions, including all 17 DOE labs;
- U.S. and world leadership in high-performance computing and computational sciences;
- Major U.S. supporter of physics, chemistry, materials sciences, and biology for discovery and for energy sciences.



Support for basic research in the physical sciences by agency.

Source: *NSF Science and Engineering Indicators 2012*

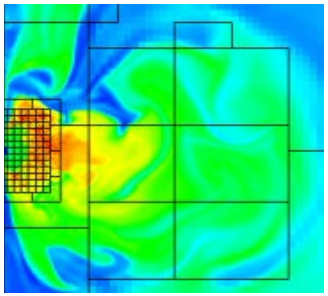
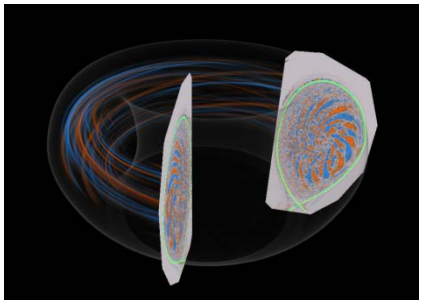
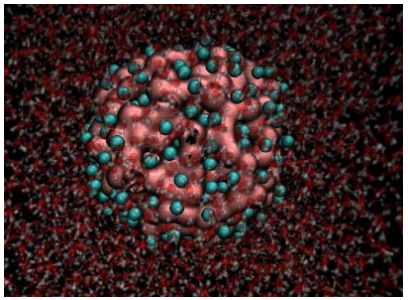
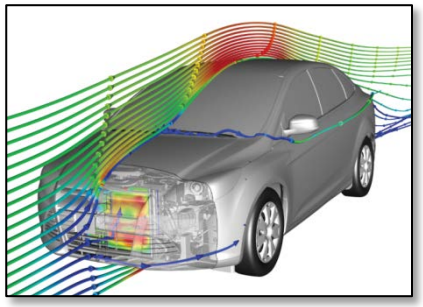
Scientific User Facilities

- The world's largest collection of scientific user facilities (aka research infrastructure) operated by a single organization in the world, used by 31,000 researchers each year.

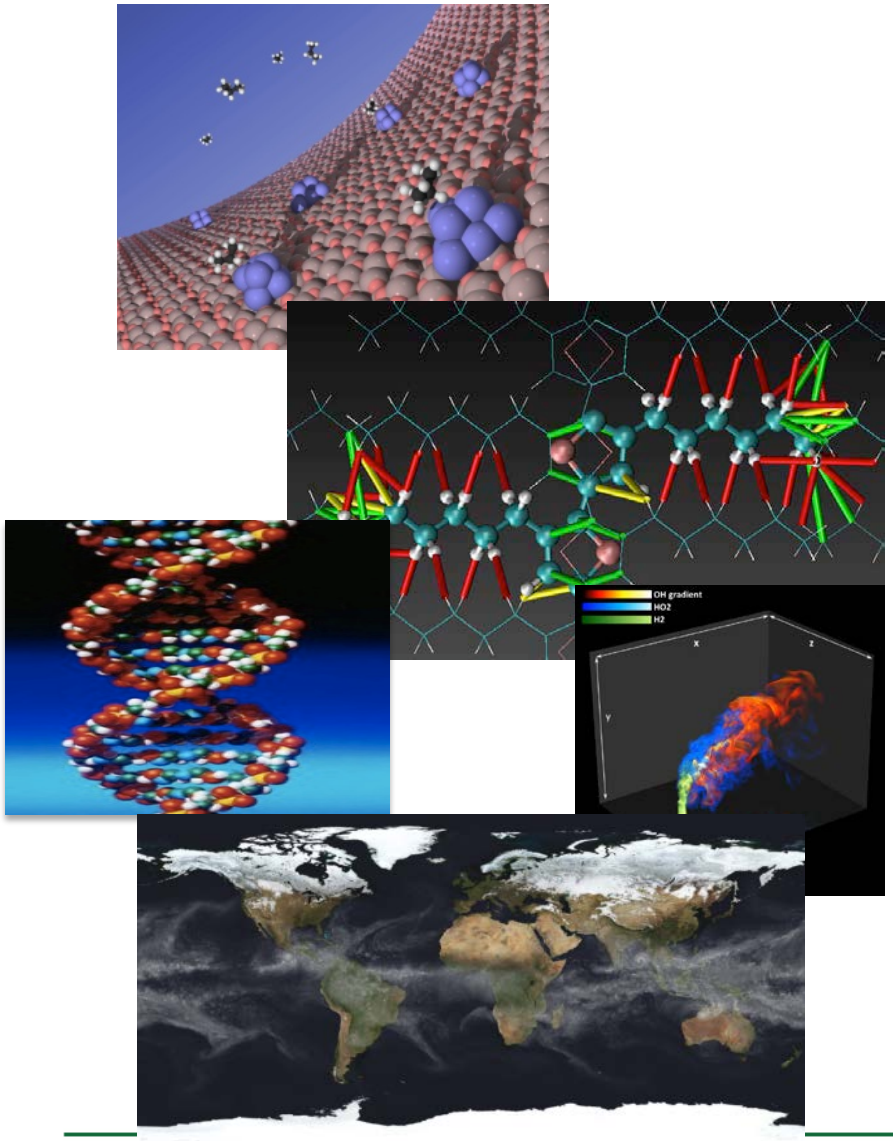
Advanced Scientific Computing Research

Computational and networking capabilities to extend the frontiers of science and technology

- **Mathematics research** to address challenges of increasing complexity within DOE's mission areas from a mathematical perspective. This requires integrated, iterative processes across multiple mathematical disciplines.
- **Computer science research** to increase the productivity and integrity of HPC systems and simulations, and support data management, analysis, and visualization techniques.
- **SciDAC partnerships** to dramatically accelerate progress in scientific computing that delivers breakthrough scientific results.
- **Exascale computing** research and development of capable exascale hardware architectures and system software, including the deployment of programming environments for energy-efficient, data-intensive applications, and engagement with HPC vendors to deliver systems that address the exascale challenges.
- **Facilities** operate with at least 90% availability while continuing planned upgrades – begin deployment of 10-40 petaflop upgrade at NERSC and continue preparations for 75-200 petaflop upgrades at each LCF.
- Continue a postdoctoral program at the ASCR facilities and provide funding for the Computational Science Graduate Fellowship to address DOE workforce needs.

ASCR Investment Priorities



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.

Budget

Office of Science FY 2016 Budget Request to Congress

(Dollars in thousands)

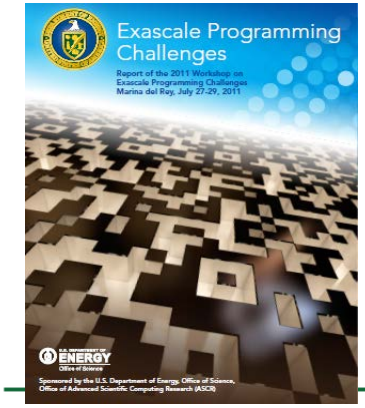
	FY 2014 Enacted Approp. (prior to SBIR/STTR)	FY 2014 Current Approp.	FY 2015 Enacted Approp.	FY 2016 President's Request	FY 2016 President's Request vs. FY 2015 Enacted Appropriation	
Advanced Scientific Computing Research	478,093	463,472	541,000	620,994	+79,994	+14.8%
Basic Energy Sciences	1,711,929	1,662,702	1,733,200	1,849,300	+116,100	+6.7%
Biological and Environmental Research	609,696	593,610	592,000	612,400	+20,400	+3.4%
Fusion Energy Sciences	504,677	495,855	467,500	420,000	-47,500	-10.2%
High Energy Physics	796,521	774,920	766,000	788,000	+22,000	+2.9%
Nuclear Physics	569,138	554,802	595,500	624,600	+29,100	+4.9%
Workforce Development for Teachers and Scientists	26,500	26,500	19,500	20,500	+1,000	+5.1%
Science Laboratories Infrastructure	97,818	97,818	79,600	113,600	+34,000	+42.7%
Safeguards and Security	87,000	87,000	93,000	103,000	+10,000	+10.8%
Program Direction	185,000	185,000	183,700	187,400	+3,700	+2.0%
SBIR/STTR (SC)	.....	128,539	.....	.....	.....	.....
Subtotal, Office of Science	**5,066,372**	**5,070,218**	**5,071,000**	**5,339,794**	**+268,794**	**+5.3%**
SBIR/STTR (DOE)	.....	64,666	.....	.....	.....	.....
Subtotal, Office of Science	**5,066,372**	**5,134,884**	**5,071,000**	**5,339,794**	**+268,794**	**+5.3%**
Use of Prior Year Balances (SBIR)	.....	-3,846	.....	.....	.....	.....
Rescission of Prior Year Balances	.....	.....	-3,262	.....	+3,262	-100.0%
Total, Office of Science	**5,066,372**	**5,131,038**	**5,067,738**	**5,339,794**	**+272,056**	**+5.4%**

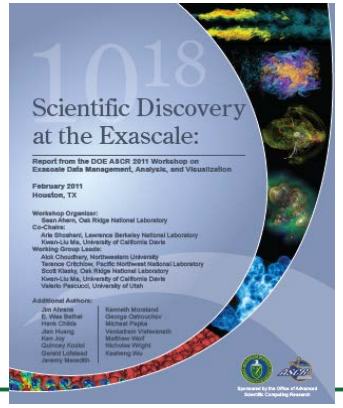
ASCR's Research

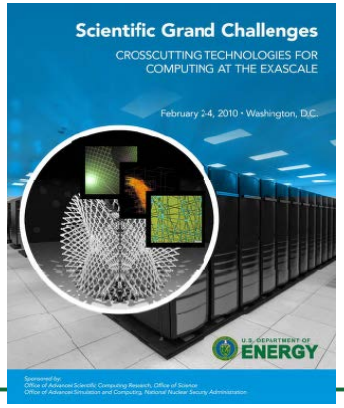
(dollars in thousands)

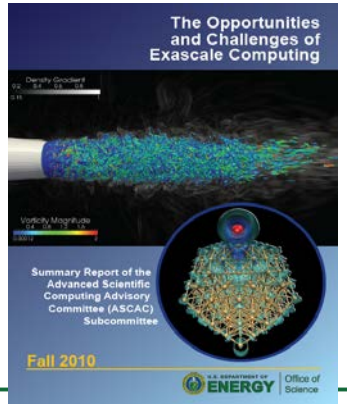
FY 2015 Current	FY 2016 Request	*FY16 vs FY15*
176,670	179,170	**+2,500**

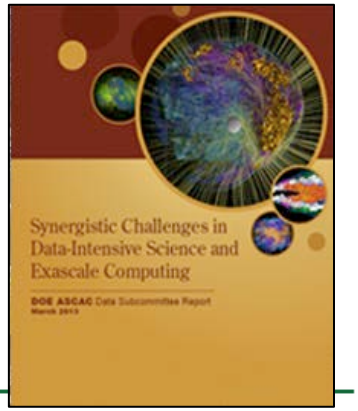
- Applied Mathematics
  - Emphasizes complex systems, uncertainty quantification, large data and exascale algorithms;
- Computer Science
  - Exascale computing (architecture, many-core, power aware, fault tolerance), operating systems, compilers, performance tools, scientific data management, integration, analysis and visualization for petabyte to exabyte data sets;
- Partnerships
  - CoDesign and SciDAC partnerships to pioneer the future of scientific applications;
- Next Generation Networks for Science
  - Tools for the future of distributed science
- Research and Evaluation Prototypes
  - Fast Forward and Design Forward partnerships with Industry and Non-Recurring Engineering for the planned facility upgrades











ASCR's Facilities

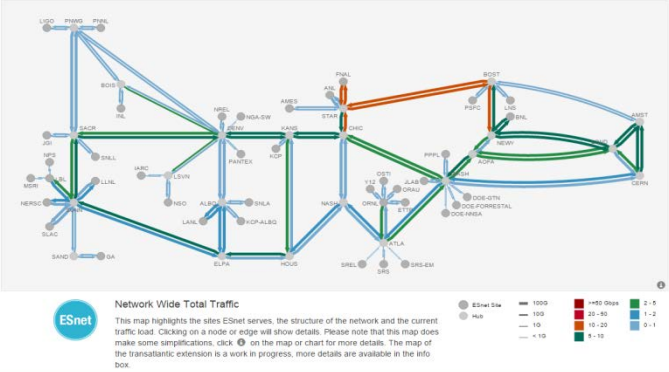
(dollars in thousands)

FY 2015 Current	FY 2016 Request	*FY16 vs FY15*
364,330	441,824	**+77,494**

Providing the Facilities – **High-End and Leadership Computing**

- **National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory**
  - Delivers high-end capacity computing to entire DOE SC research community
  - Over 5,000 users and 400 projects
- **Leadership Computing Centers at Argonne National Laboratory (ALCF) and Oak Ridge National Laboratory (OLCF)**
  - Established in response to P.L. 108-423, "Department of Energy High-End Revitalization Act of 2004"
  - Delivers highest computational capability
    - Open to national and international researchers, including industry
    - Not constrained by existing DOE or Office of Science funding or topic areas
    - Allocations based on rigorous peer and computational reviews
  - Approximately 300 users and 25-30 projects at each center, each year

Linking it all together – **Energy Sciences Network (ESnet)**



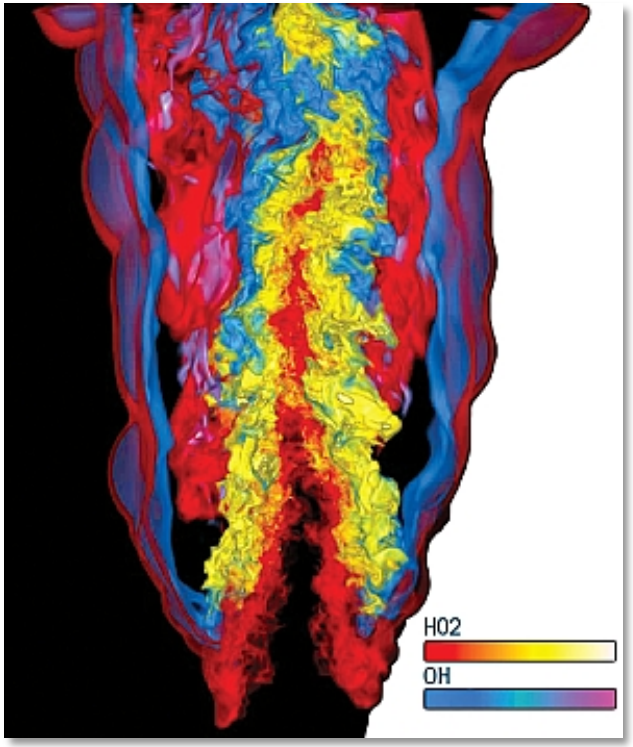
Path to the Future – **Research & Evaluation Prototypes**

Exascale Computing Initiative: Next Generation of Scientific Innovation

- **Departmental Crosscut – 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 – next-generation materials
  - Mission-focused basic science in energy – next-generation climate software
  - Use current Leadership Computing approach for users
- **The next generation of advancements will require Extreme Scale Computing**
  - 100-1,000X capabilities of today's computers with a similar physical size and power footprint
  - Significant challenges are power consumption, high parallelism, reliability
- **Extreme Scale Computing, cannot be achieved by a "business-as-usual," evolutionary approach**
  - Initiate partnerships with U.S. computer vendors to perform the required engineering, research and development for system architectures for capable exascale computing
  - Exascale systems will be based on marketable technology – Not a "one off" system
  - Productive system – Usable by scientists and engineers

(dollars in thousands, SC/ASCR portion)

FY 2015 Current	FY 2016 Request	*FY16 vs FY15*
91,000	177,894	**+86,894**



ASCR Budget Overview

	FY 2014 Current Appropriation (w/o SBIR/STTR)	FY 2015 Enacted Approp.	FY 2016 President's Request	*FY16 vs. FY15*
Advanced Scientific Computing Research				
Exascale — Applied Mathematics	47,081	49,155	49,229	+74
Exascale — Computer Science	55,835	55,767	56,842	+1,075
Exascale — Computational Partnerships (SciDAC)	46,261	46,918	47,918	+1,000
Next Generation Networking for Science	17,852	19,000	19,000	+0
SBIR/STTR	0	5,830	6,181	+351
Total, Mathematical, Computational, and Computer Sciences Research	*167,029*	*176,670*	*179,170*	*+2,500*
High Performance Production Computing (NERSC)	67,105	75,605	76,000	+395
Leadership Computing Facilities	160,000	184,637	171,000	-13,637
Exascale — Research and Evaluation Prototypes	36,284	57,329	141,788	+84,459
High Performance Network Facilities and Testbeds (ESnet)	33,054	35,000	38,000	+3,000
SBIR/STTR	0	11,759	15,036	+3,277
Total, High Performance Computing and Network Facilities	*296,443*	*364,330*	*441,824*	*+77,494*
Total, Advanced Scientific Computing Research	**463,472**	**541,000**	**620,994**	**+79,994**

Updates

- **CSGF**
- **Appointees**
- **ASCR Personnel Changes**
- **Requirements Gathering Process**
- **Exascale update**
- **CORAL Procurement**
- **NERSC/ESnet Update**
- **Secretary of Energy Advisory Board**
- **Recent ASCR Workshops**

Partnerships to Deliver Future Leaders

DOE Computational Science Graduate Fellowship (CSGF)

- **Started in 1991 to broadly train advanced computational scientists**
- **Funded by both DOE-SC/ASCR and NNSA/ASC**
- **Requires that fellows**
  - plan and follow a plan of study that transcends the bounds of traditional academic disciplines
  - participate in 12-week research experience at DOE lab
- **Benefits**
  - Up to four years of support, including full tuition and required fees paid
  - Yearly stipend of $36,000
  - Academic allowance
- **CSGF Longitudinal Study (2012)**
  - ➢ "…The generation of a DOE CSGF community of scholars and the building of collaborative networks – notably, often across generational and disciplinary lines – have been critical outcomes of the Fellowship experience." (page 18)
  - ➢ "…By linking individual elements with institutional and external realities and needs, the DOE CSGF program itself has operated to identify and involve individuals who might serve not only the field and their own professional goals, but also the national agenda and society more generally, both directly and indirectly." (page 75)

The Subcommittee believes that the CSGF is unique in its focus on Computational Science. It provides features that other Graduate research Fellowships do not, such as the Plan of Study, the Practicum, the Annual CSGF Conference and efforts to keep alumni engaged. In this regard, the CSGF is an exceptional program that produces interdisciplinary scientists uniquely qualified to address current and future computational science challenges.

2011 ASCAC Review of DOE Computational Science Graduate Fellowship Program

For Immediate Release

Professor Marc Kastner, Renowned Physicist and MIT Dean, Named President of the Science Philanthropy Alliance

Prof. Kastner will head group of funders aiming to build U.S. philanthropic support for basic science research

(Issued by The Kavli Foundation on behalf of the Science Philanthropy Alliance)

February 26, 2015

ASCR Personnel Changes

- Sandy Landsberg: Departing for DoD HPC Modernization Program
- Melea Baker: Retiring from federal service after 30 years federal service
- Robert Lindsay: Retiring from federal service (Research Division)
- Ceren Susut-Bennett: on 4-month detail to National Science Foundation

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

August 10, 2014

- Secretary posed three supplementary questions in his October 2014 letter to SEAB
- SEAB responded to the Secretary's questions in its November 2014 letter†
- The Secretary will deliver the Department's response to the SEAB in the next SEAB meeting, March 31, 2015

*http://energy.gov/sites/prod/files/2014/10/f18/SEAB%20HPC%20Task%20Force%20Final%20Report.pdf
†http://energy.gov/sites/prod/files/2015/02/f19/HPC%20Task%20Force%20Follow%20Up%20Response%20V7%20Final%2019-DEC-14_FINAL.pdf

Secretary of Energy Advisory Board – Exascale Task Force 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.

Secretary's Supplemental Questions to SEAB (1/3)

Question 1: *Can the Task Force provide an additional level of granularity on the allocations against major technology areas and their timing that regulate success in getting to the 1-10 exascale range in a decadal time frame?*

Summary of Task Force Response to Question 1: The Task Force response provides a discourse on the need to support both R&D and acquisitions and an estimate of the cost to achieve operational exascale computing. They

- envision a decade-long program will be required to achieve exascale computing, with intermediate steps, including prototypes, along the way;
- estimate that the funding profile for exascale will extend through 2024, with peaks in the range above $350 million per year but less than $400 million per year; and
- note that the cost of individual exascale computers will be in the $200-250M range, which is approximately $90M more than seen in the recent CORAL acquisitions.

Secretary's Supplemental Questions to SEAB (2/3)

Question 2: *Could the Task Force provide suggestions for what the Department could undertake to expand industrial high-end HPC use?*

Summary of Task Force Response to Question 2: The Task Force response notes the history of successful HPC partnerships in DOE, with specific mention of the DOE INCITE program and LLNL's HPC Innovation Center. The response describes two broad classes of potential industry users: 1) large industries, for which the use of large scale computational modeling, simulations, and data analysis is standard and does not require "proof of concept" to justify its use, and 2) smaller companies that would benefit from expanded use of DOE HPC but, for reasons of size (people resources), capability (financial resources), or inexperience, do not currently make significant use of high performance computing in their operations. The Task Force itemizes four specific recommendations for DOE to undertake:

- Create and support an easy to navigate DOE portal describing all publicly available computing resources and programs to access them, tools to determine the best fit to the problems and opportunities presented by the private sector, and clear instructions and guidelines on how to access the resources and programs. Specifically, each DOE facility offering such access should identify and support a single individual to serve as an initial point of contact for a new company wishing to explore access.
- Continue to support competitive programs that provide access to leading edge HPC computing at the DOE. Ensure that such awards include not only a designated amount of computing time but also ensured access to the computational and domain specific expertise in the labs that support those capabilities. Access to such programs should be through three categories:
  - Initial awards at no charge to the outside party, with priority put on new users or new applications.
  - Subsidized access to small and medium enterprises aimed at expanding the national user base of high performance computing.
  - Follow on awards to large enterprises on a full or partially subsidized pay-as-you-go basis. As an added incentive, such programs might give "credit" to large enterprises that bring new partners to a computational program.
- As part of the broader enhanced technology efforts underway at DOE, the Department should support programs leading to the commercialization of new or matured codes so that such codes are available through the ISV model to the public user community.
- The DOE should be a key partner with the university community, the national academic accreditation bodies, and the private sector in enhancing engineering and science degree programs, to ensure that graduates have the necessary background and skills needed for a future in which effective use of high performance computing will be a standard expected capability for a STEM career.

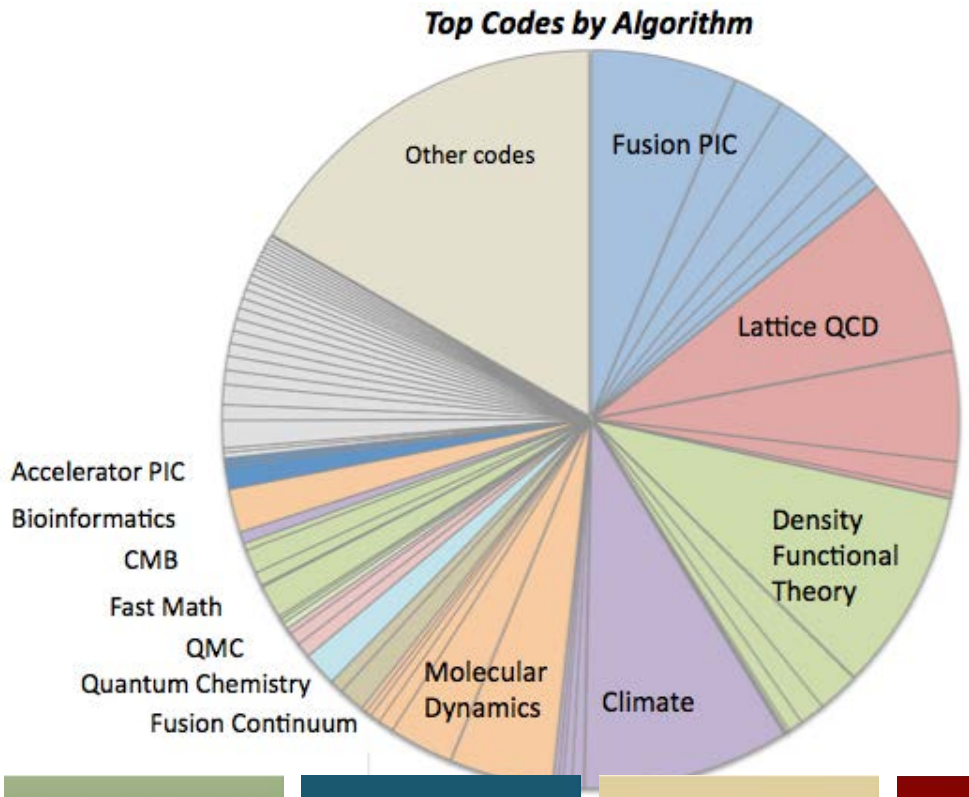
Secretary's Supplemental Questions to SEAB (3/3)

Question 3: *[Your] further thoughts on how a beyond-exascale research program (superconducting, quantum, neuromorphic…) might be structured would be appreciated.*

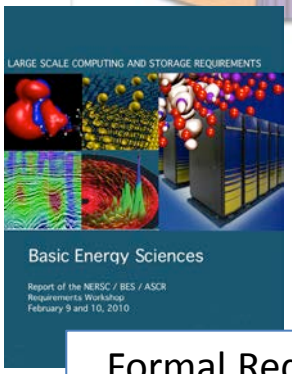
Summary of Task Force Response: The Task Force states its view that there are three promising areas of advanced high performance computing currently being researched: quantum computing, superconducting circuits, and neuromorphic computing. The Task Force recommends

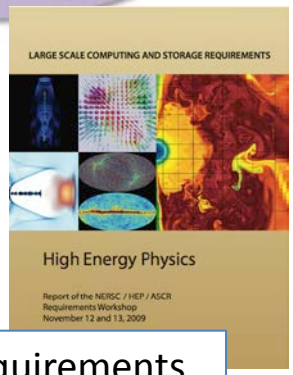
- rather than commit to specific technologies in "over-the-horizon" computational systems, DOE should invest to maintain and strengthen the computational ecosystem, including working with universities, which would allow DOE to understand what already is underway, while focusing on more advanced elements of over-the-horizon computing, including software development; and
- combining with the path to exascale, investments to sustain the advanced computing ecosystem, and to look "over the horizon" should be funded at $100-$150 million per year. Included in this amount should be $20-$25 million per year to enable DOE to stay abreast of developments being sponsored by others

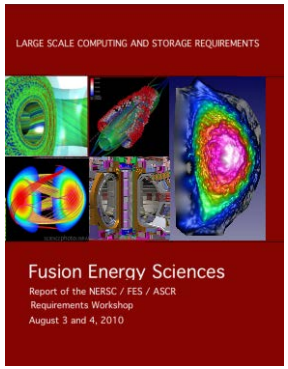
Computational Capacity is Based on Requirements

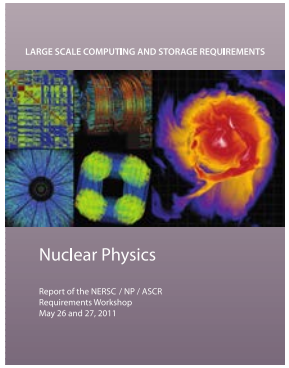


Computational Usage at NERSC (2014)









Formal Requirements Gathering Process

Objectives of Exascale Requirements Review

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

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

- Identify continuum of computing needs from HPC to Leadership. All three ASCR Leadership and HPC facilities are involved.
- Include modeling and simulation, scientific user facilities needs, data needs, and near real time needs.
- Information gathered will inform the requirements for an exascale ecosystem including the exascale system, network needs, data infrastructure, software support, and user services.

Communicate to DOE SC scientists the known/fixed characteristics of upcoming compute system in the 2020-2025 timeframe.

Strengthen and inform interactions between HPC facility experts and scientists as well as ASCR and SC domain office.

Implementation of Exascale Requirements Review

Series of workshops, one per domain program (hybrid of NERSC requirements reviews and Scientific Grand Challenges)

- **Location:** Washington DC area
- **Program Committee:** Representative community leaders from SC domain program office and ASCR facility staff
- **Attendance**: ~50 attendees including DOE program managers, DOE SC community representatives, ASCR supported applied mathematicians and computer scientists and a small number of Postdocs and senior CSGF fellows

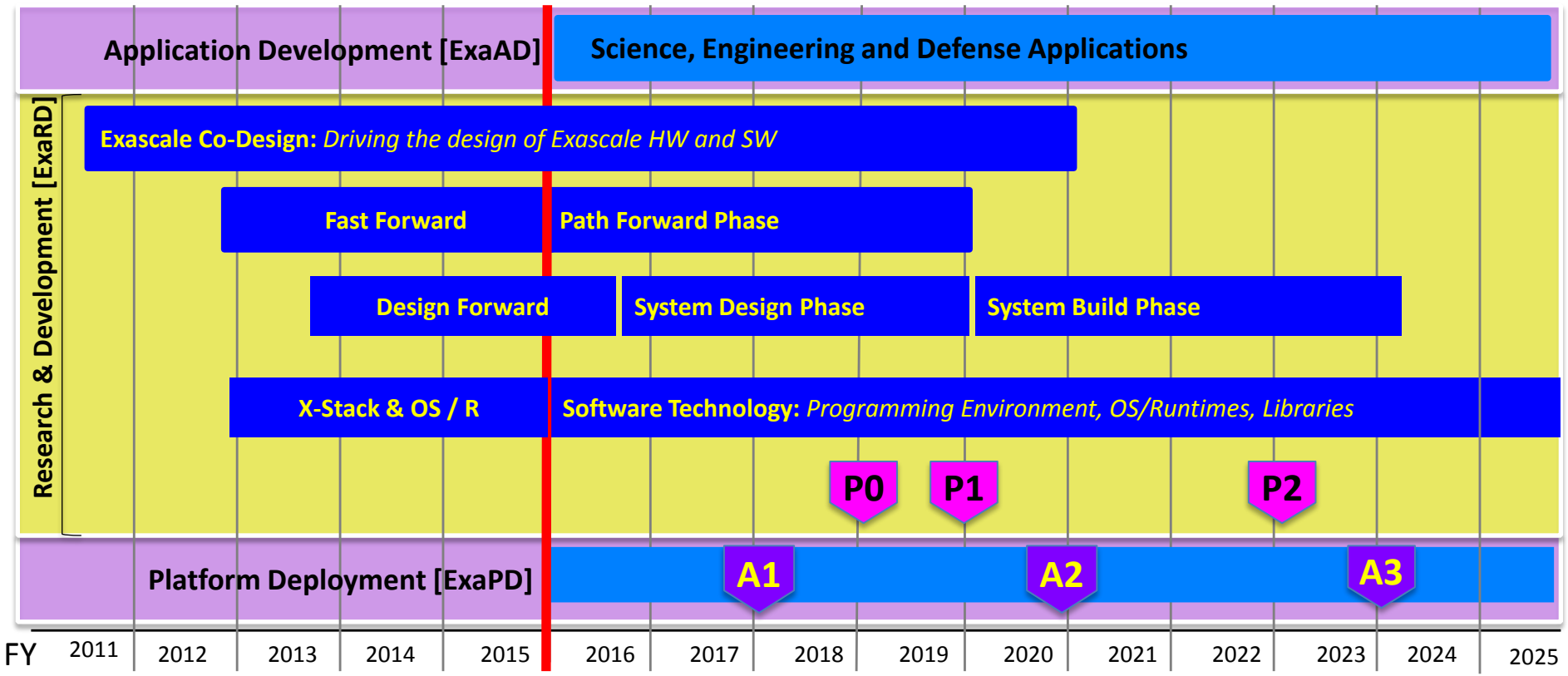
Proposed Schedule*

June 2015	HEP
September 2015	BES
December 2015	FES
April/March 2016	BER
June 2016	NP
September 2016	ASCR

- **Agenda**: Plenary session and themed breakout sessions determined by program committee
- **Pre-meeting homework**: Templates will be developed and provided to chairs and attendees of breakout session for discussing and documenting case studies
- **Output**: Summary workshop report written for each workshop.

*Dates under discussion with domain programs

Exascale Computing Initiative (ECI) Timeline



P0	Node Prototype	P1	Petascale Prototype	P2	Exascale Prototype
A1	CORAL	A2	APEX	A3	Exascale

Path Forward in CY-2015

- February 2 – FY-2016 budget is released to Congress
- February-May – Continue to refine requirements to be used in FOAs, RFPs, and ECI goals
- February-March – DOE-Congressional hearings and briefings

- March-June – ASCAC review of ECI
- March – initiate “rapid requirements assessments” needed for FY17 budget
- April-May – Conduct ECI-vendor meetings
- April 30 – ECI CD-0 approval
- May-June – Prepare FY 2017 ECI budget request; reviews up through S-1
- July – Conduct second external agency review of ECI
- July 31 – “Red team” review of ECI CD-1 package (with detailed baseline schedule and cost)
- July 31 – Complete “rapid” assessments needed for FY17 budget
- July-August – Finalize FY 2017 ECI budget request within DOE
- September – Submit FY 2017 budget to OMB
- October – release FY 2016 FOAs (pending passage of appropriation)
- October-December – DOE/OMB discussions and FY17 budget resolution

CORAL Collaboration ORNL, ANL, LLNL)

Objective – Procure three leadership computers to be sited at Argonne, Oak Ridge and Lawrence Livermore in 2017-8. Two of the contracts have been awarded with the Argonne contract in process.

Current DOE Leadership Computers

Titan (ORNL) 2012 - 2017

Sequoia (LLNL) 2012 - 2017

Mira (ANL) 2012 - 2017

Leadership Computers: The RFP seeks >100 PF, 2 GB/core main memory, local NVRAM, and science performance 4x-8x Titan or Sequoia

Approach

- **Competitive process -** one RFP (issued by LLNL) leading to two R&D contracts and three computer procurement contracts
- For risk reduction and to meet a broad set of requirements, **two architectural paths will be selected and Oak Ridge and Argonne must choose different architectures**
- **Once Selected, multi-year lab-awardee relationship to co-design computers**
- **Both R&D contracts** jointly managed by the three Labs
- **Each lab manages and negotiates its own computer procurement contract,** and may exercise options to meet their specific needs
- **Saves money for DOE and vendors** – One procurement process for DOE and one proposal to write for vendors.

ASCR Computing Upgrades At a Glance

System attributes	NERSC Now	OLCF Now	ALCF Now	*NERSC Upgrade*	*OLCF Upgrade*	*ALCF Upgrade*
Name/Planned Installation	**Edison**	**TITAN**	**MIRA**	***Cori 2016***	***Summit 2017-2018***	***Aurora 2018-2019***
System peak (PF)	2.4	27	10	*>30*	*150*	*>150*
Peak Power (MW)	3	8.2	4.8	*<3.7*	*10*	*~13*
System memory per node	64 GB	38 GB	16 GB	*64-128 GB DDR4 16 GB High Bandwidth*	> 512 GB (High Bandwidth memory and DDR4)	TBA
Node performance (TF)	0.460	1.452	0.204	*>3*	*>40*	*>15 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 & mulitple Nvidia Voltas GPUS*	*TBA*
System size (nodes)	5,200 nodes	18,688 nodes	49,152	*9,300 nodes 1,900 nodes in data partition*	*~3,500 nodes*	*~50,000 nodes*
System Interconnect	Aries	Gemini	5D Torus	*Aries*	*Dual Rail EDR-IB*	*TBA*
File System	17.6 PB, 168 GBs, Lustre®	32 PB, 1 TB/s, Lustre®	*GPFS™*	*28 PB, 744 GB/sec , Lustre®*	*120 PB, 1 TB/s, GPFS™*	*TBA*

CORAL acquisitions

CORAL Node/Rack Layout – ORNL Summit Computer

CORAL rack layout

- 18 nodes
- **779 TF**
- 11 TB RAM
- **55 KW**

CORAL System

- ~200 racks

NERSC-8 (Cori) Delivery in 2016

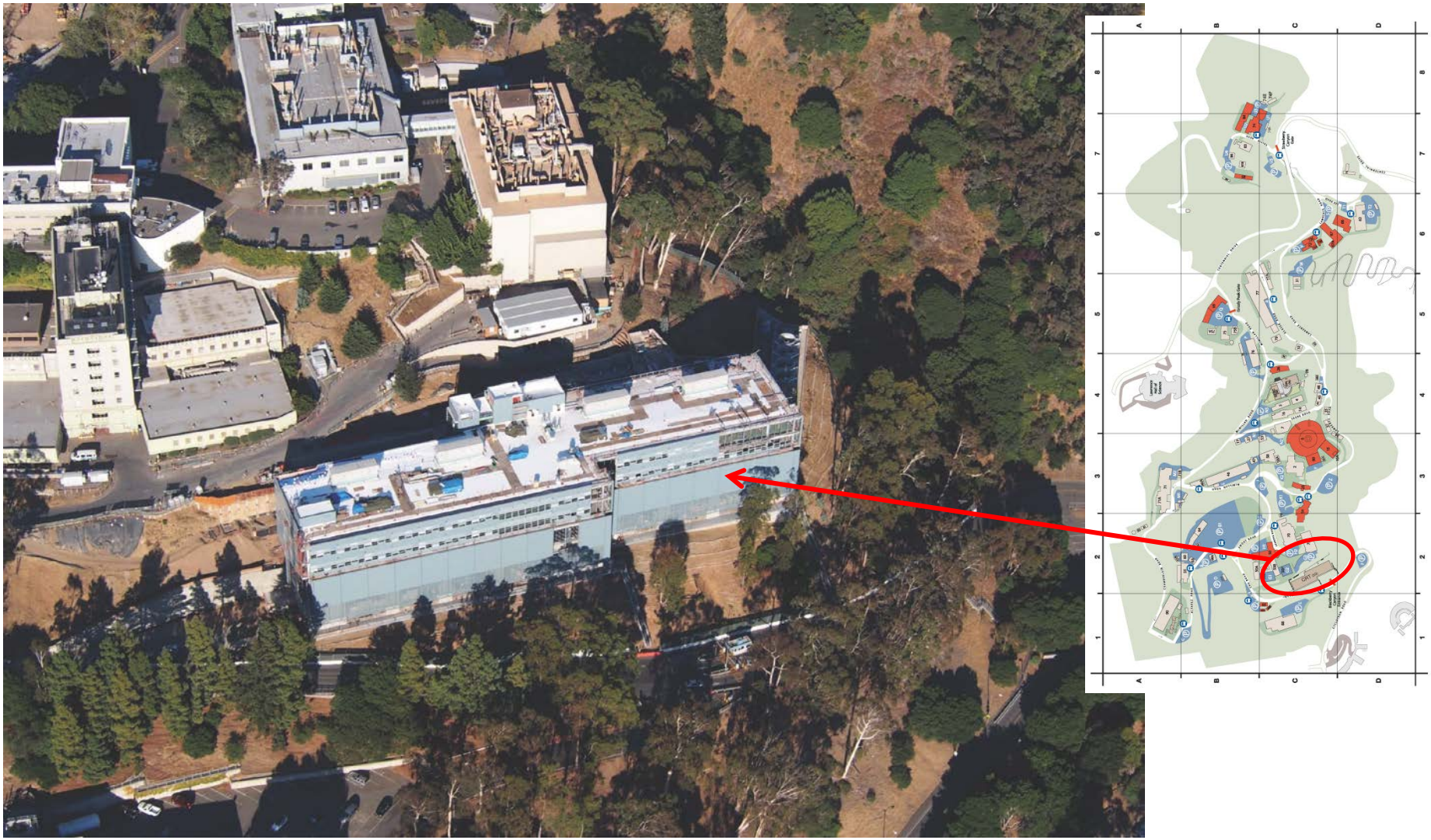
- 64-Cabinet Cray XC System
  - 10x Hopper sustained performance using NERSC SSP metric
  - ~9,300 'Knights Landing' compute nodes
    - Self-hosted (not an accelerator)
    - Greater than 60 cores per node with four hardware threads each
    - 64-128 GB memory per node
    - High bandwidth on-package memory
  - ~1,900 'Haswell' compute nodes
    - Data partition
  - Aries Interconnect (proprietary Cray – same as on Edison)
- Lustre File system
  - 28 PB capacity, 432 GB/sec peak performance
- NVRAM "Burst Buffer" for I/O acceleration
- Delivery in mid-2016 – installation in new LBNL Computational Research & Theory facility

NERSC-8 system named after Gerty Cori (1896 – 1957)

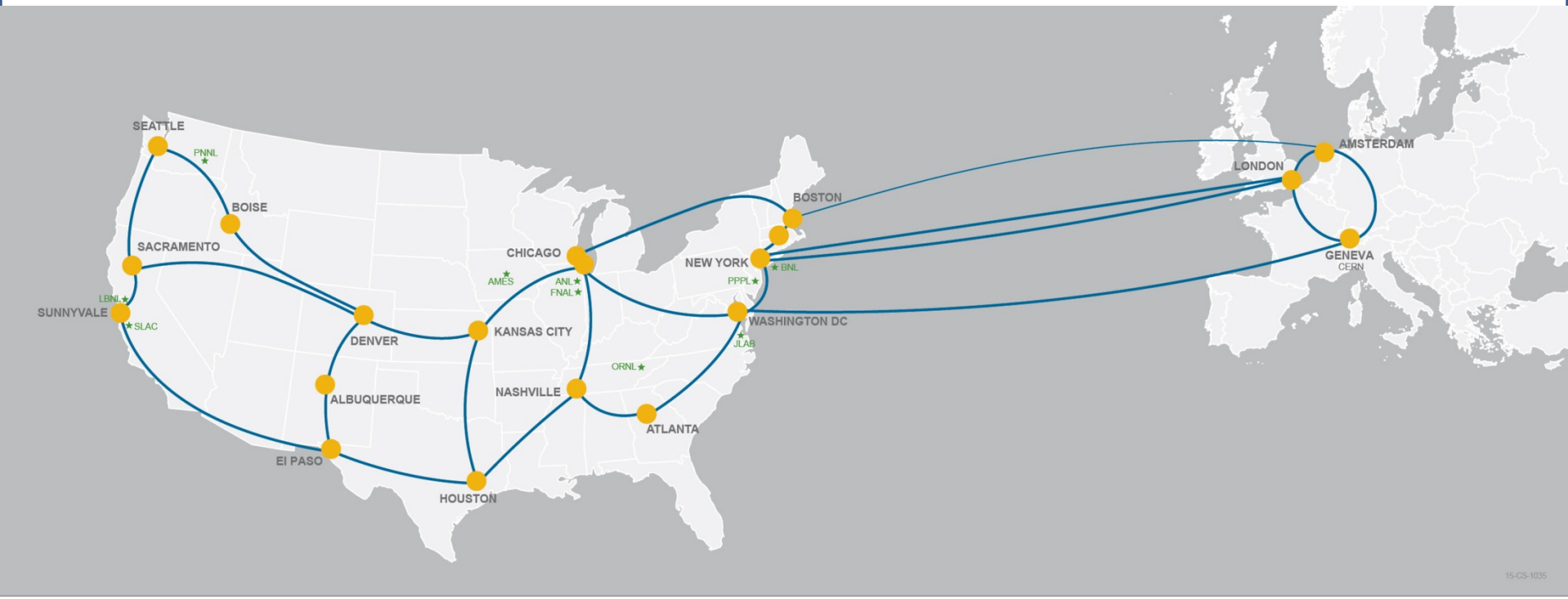
- First American woman to be awarded a Nobel Prize in science (1947)
- Born in Prague; U.S. naturalized 1928
- Shared the Nobel Prize in Physiology or Medicine with her husband and Bernardo Houssay
- Recognized for work involving enzyme chemistry in carbohydrates: how cells produce and store energy.

- Breakdown of carbohydrates and mechanism of enzyme action are of fundamental importance in renewable bioenergy (cf. DOE Complex Carbohydrate Research Center)

LBNL Computational Research and Theory Building



ESnet – Stay tuned for Dr. Greg Bell's talk …



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)

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

- CMOS lithographic feature sizes are approaching fundamental limits
  - Currently at 22 nm (both Intel and Nvidia)
  - 11 nm is projected for ~2015 (both Intel and Nvidia)
    - However, gate lengths may be smaller than 6 nm – corresponding gate dielectric thickness may reach a monolayer or less
  - The Intel roadmap reaches beyond 11 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 technoligies, including molecular electronics, spin-based computing, single-electron devices, and graphene have been proposed
    - At scales of ~10 nm, quantum tunneling is expected to become significant
  - Capital costs for tooling are increasing dramatically as feature sizes shrink
- Options:
  - Computing using superconducting technologies
  - Quantum computing
  - Neuromorphic computing
  - Probabilistic computing
  - ???

Considerable R&D required

Recent ASCR Workshops

DOE/ASCR Workshop on Quantum Computing in Scientific Applications

Date: February 17-18, 2015
Venue: DoubleTree by Hilton Hotel, Bethesda MD
Contact: Dr. Ceren Susut-Bennett, DOE/SC/ASCR, ceren.susut-bennett@science.doe.gov

The goal of the workshop is to assess the viability of quantum computing technologies to meet the computational requirements in support of DOE's science and energy mission and to identify the potential impact of these technologies.

Research into quantum computing technologies is making rapid progress and it is important for the Office of Advanced Scientific Computing Research (ASCR) to understand the utilization of these new technologies for DOE-relevant applications and their impact on conventional computing systems.

The workshop will explore the following topics:

Workshop Goals

Research into quantum computing technologies is making rapid progress and it is important for ASCR to understand the utilization of these new technologies for DOE-relevant applications and their impact on conventional computing systems. The goal of the workshop is to explore the following topics:

1. Mission relevance: What aspects of DOE's science mission are suitable for quantum computing? What are the early tests that will demonstrate viability, or lack thereof, for the DOE's mission in fundamental and applied sciences?
2. Impact on Computing: How will quantum computing improve the properties of the computation with respect to conventional contemporary computational systems? Such attributes include, but are not limited, to performance, capacity, power, cost, generality and programmability.
3. Challenges: What are the challenges in adopting quantum computing technologies and developing the required infrastructure? What algorithm/application bottlenecks need to be solved before a quantum enabled system can be used for mission critical applications? What can ASCR do to mitigate these challenges?

http://www.csm.ornl.gov/workshops/ascrqcs2015/index.html

Recent, Related DOE/NNSA Community Activities

- Workshop on Materials Opportunities for Quantum Computing,* October 7-8, 2014, LANL
- Grand Challenges at the Intersections of QIS, Particle Physics, and Computing, December 11, 2014, DOE/HEP
- NNSA Workshop on Applications of Quantum Computing, February 5-6, 2015, SNL (organized by LANL)
- DOE/ASCR Workshop on Quantum Computing in Scientific Applications, Date: February 17-18, 2015

*Community organized

Quantum Information Science is Broad and Multidisciplinary

- **Spans multiple disciplines**
  - Computer science, applied mathematics, networking, information science
  - High-energy physics (advances in quantum theory)
  - Materials sciences (new materials)
- **Has many, conceivable applications**
  - Quantum simulation
  - Sensors
  - Cryptography
  - Communications, networking
  - Metrology/measurement, accurate timekeeping, …
  - …
- **Quantum theory is evolving**
  - new understanding of entanglement and information theory
- **Practical quantum computers require new technologies**
  - New materials for quantum devices
  - qubit manipulation, error correction
  - System integration
  - Software
  - …

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

COV Charge – Next-Generation Networks for Science

Department of Energy
Washington, DC 20585

MAR 2 0 2015

Dr. Roscoe Giles, ASCAC Chair
Department of Electrical and Computer
Engineering
Boston University
8 St. Mary's Street
Boston, MA 02215

Dear Dr. Giles:

Thank you for the excellent Committee of Visitors (COV) review of the Scientific Discovery through Advanced Computing (SciDAC) program. The Office of Advanced Scientific Computing Research (ASCR) has already undertaken changes to respond to the recommendations of the COV and improve the management of this important program. The full program response and action plan is posted on the ASCAC website (http://www.sc.doe.gov/ascr/ASCAC/Reports.html).

To help the research communities make efficient and effective use of current and future computing capabilities, ASCR also supports a basic research program in Networking. To ensure the integrity of this research program, I am asking the Advanced Scientific Computing Advisory Committee (ASCAC) to assemble a Committee of Visitors (COV) to review the management processes for the Next Generation Networking for Science (NGNS) elements of the ASCR program. A report will be expected at the November 2015 ASCAC meeting.

The COV should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. The Committee should assess the operations of the Networking programs during the fiscal years 2011, 2012, 2013 and 2014. The panel may examine any files from this period for both DOE laboratory projects and university projects. The Committee will be provided with background material on the program prior to the meeting.

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

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

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2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
   (a) the breadth and depth of portfolio elements, and
   (b) the degree to which the program is anticipating and addressing emerging challenges from large-scale scientific facilities and collaborations in support of the DOE missions, and
   (c) the national and international standing of the program with regard to other computer science research programs that are also focused on high performance networking tools and middleware for science.

If you, or the COV chair, have any questions, please contact Christine Chalk, Designated Federal Official for ASCAC at 301-903-5152 or by e-mail at christine.chalk@science.doe.gov.

I appreciate ASCAC's willingness to undertake this important activity.

Sincerely,

Patricia M. Dehmer
Acting Director
Office of Science

BACKUPS

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)

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.