



U.S. DEPARTMENT OF
ENERGY

Office of
Science

View from Germantown

Advanced Scientific Computing Research Update

Barbara Helland, Associate Director

September 30, 2022

Some ASCAC Agenda Details

- ▶ ASCR RESEARCH PRIORITIES – *Ceren Susut, ASCR*
- ▶ GENERAL MOTORS (GM) AT EXASCALE - *Paul Krajewski, General Motors*
- ▶ ASCAC DISCUSSION – *Dan Reed, ASCAC Chair*
- ▶ EXASCALE UPDATE – *Lori Diachin, Lawrence Livermore National Laboratory and William Hart, Sandia National Laboratories*
- ▶ ESNET-6 UPDATE – *Inder Monga, Lawrence Berkeley National Laboratory*
- ▶ SUBCOMMITTEE REPORTS
 - ▶ DOE-NCI COLLABORATIONS – *Tony Hey, ASCAC*
 - ▶ INTERNATIONAL BENCHMARKING – *Jack Dongarra, ASCAC*

Advancing DEI in SC Business Practices

- SC Programs initiated several new practices with the launch of the Reaching a New Energy Science Workforce (RENEW) initiative this year:
 - Community Listening Sessions to identify barriers to participation in SC program opportunities.
 - Incorporating direct elements of the scope of proposals and allowable costs to directly address barriers to participation.
 - Post-FOA announcement webinars to answer community questions.
 - A requirement for a *Recruitment and Inclusion Plan* as part of the application to promote intentional support for diverse and inclusive research and training environments.
 - The *Recruitment and Inclusion Plan* was evaluated in the merit review process under its own criterion.

SC plans to expand upon these new practices and requirements in FY 2023.

ASCR BUDGET UPDATES

- ▶ FY2023 President's Budget Request (PBR)
- ▶ F2023 Senate Marks

ASCR - FY 2023 President's Request

(Dollars in thousands)

	FY 2021	FY 2022	FY 2023	FY 2023 Request vs		FY 2023 Request vs	
	Enacted	Enacted	Request	FY 2022 Enacted		FY 2021 Enacted	
Advanced Scientific Computing Research							
Applied Mathematics Research	48,570	51,048	71,938	20,890	40.92%	23,368	48.11%
Computer Sciences Research	46,827	49,773	70,326	20,553	41.29%	23,499	50.18%
Computational Partnerships	76,194	79,456	97,861	18,405	23.16%	21,667	28.44%
Advanced Computing Research	88,274	105,723	113,598	7,875	7.45%	25,324	28.69%
Energy Earthshot Research Centers	25,000	25,000	...	25,000	...
Mathematical, Computational, and Computer Sciences Research	259,865	286,000	378,723	92,723	32.42%	118,858	45.74%
High Performance Production Computing	113,786	120,000	115,033	-4,967	-4.14%	1,247	1.10%
Leadership Computing Facilities	381,075	410,000	407,772	-2,228	-0.54%	26,697	7.01%
High Performance Network Facilities and Testbeds	91,329	90,000	90,213	213	0.24%	-1,116	-1.22%
High Performance Computing and Network Facilities	586,190	620,000	613,018	-6,982	-1.13%	26,828	4.58%
17-SC-20 SC Exascale Computing Project	168,945	129,000	77,000	-52,000	-40.31%	-91,945	-54.42%
Total Advanced Scientific Computing Research	1,015,000	1,035,000	1,068,741	33,741	3.26%	53,741	5.29%

2022 Inflation Reduction Act: ASCR - \$163,791,000 for projects

ASCR's FY2023: Senate Markup

- ▶ The Committee recommends \$1,077,000,000 for Advanced Scientific Computing Research (ASCR).
- ▶ The Committee strongly supports ASCR's leadership in emerging areas relevant to the Department's mission, including artificial intelligence and quantum information science. The committee commends ASCR's pursuit of machine learning tools for scientific applications and its support for the development of algorithms for future deployment quantum computers.
- ▶ **High Performance Computing and Network Facilities.— not less than**
 - ▶ \$178,000,000 for the Argonne Leadership Computing Facility,
 - ▶ \$263,000,000 for the Oak Ridge Leadership Computing Facility
 - ▶ \$130,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory.
 - ▶ \$91,000,000 to support necessary infrastructure up-grades and operations for ESnet.
- ▶ **Mathematical, Computational, and Computer Sciences Research.—**
 - ▶ Not less than \$280,000,000 for Mathematical, Computational, and Computer Sciences Research.
 - ▶ \$20,000,000 for CSGF

ASCR's FY2023 Senate Markup (cont.)

- ▶ The Committee supports the **Center for Advanced Mathematics for Energy Research Applications (CAMERA)** and encourages the Department to support the creation of a crosscutting research program that leverages applied math, computer science and computational science to deliver artificial intelligence research, development, and deployment to increase the scientific productivity of the user facilities.
- ▶ The Department is encouraged to **explore the viability of photonic quantum computing**, in coordination with other federal agencies. The Department is encouraged to **consider mechanisms to provide access to ion trap quantum computing resources**, particularly with the ability to integrate with existing high-performance computing resources.

FY 2022 Congressional Action: A closer look at the House and Senate Marks

(\$ in thousands)

	FY2022 Enacted	FY2023 Request	House Mark Language (not less than)	Senate Mark Language (not less than)
ASCR	1,035,000	1,068,730	1,050,000	1,077,000
ALCF	152,955	159,047	170,000	178,000
OLCF	228,120	249,066	250,000	263,000
NERSC	120,000	115,033	120,000	130,000
Esnet	90,000	90,213	90,000	91,000
Total Research	286,000	378,723	>340,000 Including \$15M- \$40M for memory research	>280,000. including \$20M for CSGF
Exascale	129,000	77,000	77,000	77,000

Chips and Science Act: ASCR authorization for FY 2023: \$1,126,950

- ▶ Chips and Science Act

ASCR FY2022 Chips and **Science** Act (Section 10104)

▶ **Authorization of Current Programs**

- ▶ The Director shall carry out, in coordination with academia and relevant public and private sector entities, a research, development and demonstration program –
- ▶ (1) to steward **applied mathematics, computational science, and computer science research** relevant to the **missions of the Department** and the **competitiveness of the United States**;
- ▶ (2) to develop modeling, simulation, and other computational tools relevant to other scientific disciplines and to the **development of new energy technologies and other technologies**;
- ▶ (3) to **advance computing and networking capabilities for data-driven discovery**; and
- ▶ “(4) to **develop advanced scientific computing hardware and software tools** for science and engineering.”;

COORDINATION.—The Under Secretary for Science shall ensure the coordination of the activities of the Department, including activities under this section, to determine and meet the computational and networking research and facility needs of the Office of Science and all other relevant energy technology and energy efficiency programs within the Department and with other Federal agencies as appropriate.

ASCR FY2022 Chips and **Science** Act (Section 10104)

- ▶ Authorization of Current Programs (continued)
- ▶ The Director shall carry out activities to develop, test, and support –
 - ▶ “(A) **mathematics, statistics, and algorithms for modeling complex systems** relevant to the missions of the Department, including on advanced computing architectures; and
 - ▶ “(B) **tools, languages, programming environments, and operations for high-end computing** systems (as defined in section 2 of the American Super Computing Leadership Act of 2017 (15 U.S.C. 5541)).
- ▶ COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP
- ▶ Support the Computational Science Graduate Fellowship program in order **to facilitate collaboration between graduate students and researchers at the National Laboratories**, and contribute to the **development of a diverse and inclusive computational workforce to help advance research in all areas of computational science** relevant to the mission of the Department, including quantum computing.

ASCR FY2022 Chips and **Science** Act (Section 10104)

- ▶ Authorization of Current Programs (continued)
- ▶ **ENERGY SCIENCES NETWORK**
- ▶ The Secretary shall ensure the following capabilities:
 - ▶ (A) To provide high bandwidth scientific networking across the continental United States and the Atlantic Ocean.
 - ▶ (B) To ensure network reliability.
 - ▶ (C) To protect the network infrastructure from cyberattacks.
 - ▶ (D) To manage transport of exponentially increasing levels of data from the Department's National Laboratories and sites, user facilities, experiments, and sensors.
 - ▶ (E) To contribute to the integration of heterogeneous computing frameworks and systems.

ASCR FY2022 Chips and **Science** Act (Section 10104)

- ▶ Authorization of Current Programs (continued)
 - ▶ **Balanced Portfolio** within the advanced scientific computing research and development program that supports robust investment in—
 - ▶ “(i) applied mathematical, computational, and computer sciences research needs relevant to the mission of the Department, including foundational areas that are critical to the advancement of energy sciences and technologies and new and emerging computing technologies; and
 - ▶ “(ii) associated high-performance computing hardware and facilities.

ASCR FY2022 Chips and **Science** Act (Section 10104)

- ▶ Authorization of New Programs

- ▶ **EXASCALE ECOSYSTEM SUSTAINMENT.—**

- ▶ SENSE OF CONGRESS.—It is the sense of Congress that the Exascale Computing Project has successfully created a broad ecosystem that provides shared software packages, novel evaluation systems, and applications relevant to the science and engineering requirements of the Department, and that such products must be maintained and improved in order that the full potential of the deployed systems can be continuously realized.

- ▶ Sustain and evolve the ecosystem to ensure that the **exascale software stack and other research software will continue to be maintained, hardened, and otherwise optimized for long-term use on exascale systems and beyond** and reliable availability to the user community.

ASCR FY2022 Chips and **Science** Act (Section 10104)

▶ Authorization of New Programs (continued)

▶ **ADVANCED COMPUTING PROGRAM.—**

- ▶ Establish a program to develop and implement a strategy for achieving computing systems with capabilities beyond exascale computing systems.
 - ▶ (A) maintain foundational research programs in mathematical, computational, and computer sciences focused on new and emerging computing needs within the mission of the Department, including post-Moore's law computing architectures, novel approaches to modeling and simulation, artificial intelligence and scientific machine learning, quantum computing, edge computing, extreme heterogeneity, including potential quantum accelerators, and distributed high-performance computing;
 - ▶ (B) retain best practices and maintain support for essential hardware, applications, and software elements of the Exascale Computing Program that are necessary for sustaining the vitality of a long-term capable software ecosystem for exascale and beyond; and
 - ▶ (C) develop a Department-wide strategy for balancing on-premises and cloud-based computing and scientific data management.

▶ **GUIDANCE ON MITIGATION OF BIAS IN HIGH-PERFORMANCE COMPUTING**

In leveraging high-performance computing systems for research purposes, including through the use of machine learning algorithms for data analysis and artificial intelligence, The Secretary shall issue, and ensure adherence to, guidance for the Department, the National Laboratories, and users as to how those capabilities should be employed in a manner that mitigates, and to the maximum extent practicable, avoids harmful algorithmic bias.

ASCR FY2022 Chips and **Science** Act (Section 10104)

- ▶ Authorization of New Programs (continued)

- ▶ **ARCHITECTURAL RESEARCH IN HETEROGENEOUS COMPUTING SYSTEMS.--**

Research and development in heterogeneous and reconfigurable computing systems to expand understanding of the potential for heterogeneous and reconfigurable computing systems to deliver high performance, high efficiency computing for Department mission challenges. The program shall include research and development that explores the convergence of big data analytics, simulations, and artificial intelligence to drive the design of heterogeneous computing system architectures.

- ▶ **COORDINATION.**—In carrying out the program described in paragraph (1), the Secretary shall ensure coordination between research activities undertaken by the Advanced Scientific Computing Research program and materials research supported by the Basic Energy Sciences program within the Office of Science.

ASCR FY2022 Chips and **Science** Act (Section 10104)

▶ Authorization of New Programs (continued)

▶ **ENERGY EFFICIENT COMPUTING PROGRAM**

▶ Fundamental research, development, and demonstration of energy efficient computing and data center technologies relevant to advanced computing applications, including high-performance computing, artificial intelligence, and scientific machine learning.

▶ (i) establish a partnership for National Laboratories, industry partners, and institutions of higher education for codesign of energy efficient hardware, technology, software, and applications across all applicable program offices of the Department, and provide access to energy efficient computing resources to such partners;

▶ “(ii) develop hardware and software technologies that decrease the energy needs of advanced computing practices, including through data center codesign;

▶ “(iii) consider multiple heterogeneous computing architectures in collaboration with the program established under sub-section (g), including neuromorphic computing, persistent computing, and ultrafast networking; and

▶ “(iv) provide, as appropriate, on a competitive, merit-reviewed basis, access for researchers from institutions of higher education, National Laboratories, industry, and other Federal agencies to the energy efficient computing technologies developed pursuant to clause (i).

Amendments to the National Quantum Initiative Act

- ▶ Definitions: The term 'quantum network infrastructure' means any facility, expertise, or capability that is necessary to enable the development and deployment of scalable and diverse quantum network technologies.
- ▶ Sec. 403. Department of Energy Quantum Network Infrastructure Research and Development Program:
 - ▶ The Secretary shall carry out a research, development and demonstration program to accelerate innovation in quantum network infrastructure in order to –
 - 1) Facilitate the advancement of distributed quantum computing systems through the internet and intranet
 - 2) Improve the precision of measurements of scientific phenomena and physical imaging technologies
 - 3) Develop secure national quantum communication technologies and strategies
 - 4) Demonstrate quantum networking utilizing the Department of Energy's Energy Science Network User Facility
 - 5) Advance the relevant domestic supply chains, manufacturing capabilities and associated simulations and modeling capabilities...

Amendments to the National Quantum Initiative Act (cont.)

- ▶ Sec. 404 Department of Energy Quantum User Expansion for Science and Technology program
 - ▶ The Secretary shall establish and carry out a program, to be known as the 'Quantum User Expansion for Science and Technology or QUEST program', to encourage and facilitate access to United States quantum computing hardware and quantum computing clouds for research purposes –
 - 1) To enhance the United States quantum research enterprise
 - 2) To educate the future quantum computing workforce;
 - 3) To accelerated the advancement of United States quantum computing capabilities; and
 - 4) To advance the relevant domestic supply chains, manufacturing processes, and associated simulation or modeling capabilities...



S. Scott Collis (1967 – 2022)



Scott received his B.S. in Aerospace Engineering summa cum laude from the University of Kansas while participating in a Cooperative Education Program at McDonnell Douglas in St. Louis, and earned his M.S. and Ph.D. in Mechanical Engineering from Stanford University. Scott's impactful professional career began as an assistant professor of Mechanical Engineering at Rice University in Houston, followed by nearly twenty years of distinguished service at Sandia National Laboratories in Albuquerque, with his last leadership position as Director of Computing Research.

Since 2017, Scott served as Sandia's Director and Program Executive for both the NNSA Advanced Simulation and Computing (ASC) and the DOE Office of Science ASCR programs.

Scott also focused on building greater ties to major U.S. industry partners as well as new opportunities for computing in energy and climate applications. He also pushed new opportunities in advanced computing, including quantum, neural-inspired, and other non-conventional computing concepts.

A public celebration of Scott's life was held on September 24, 2022, in Albuquerque.

Backup

ASCR's FY2023: House Markup

- ▶ The Advanced Scientific Computing Research (ASCR) program develops and hosts some of the world's fastest computing and network capabilities to enable science and energy modeling, simulation, and research.
- ▶ **High Performance Computing and Network Facilities.— not less than**
 - ▶ \$170,000,000 for the Argonne Leadership Computing Facility,
 - ▶ \$250,000,000 for the Oak Ridge Leadership Computing Facility
 - ▶ \$120,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory.
 - ▶ \$90,000,000 to support necessary infrastructure up-grades and operations for ESnet.
- ▶ The Department is directed to support continued planning and design for the **High-Performance Data Facility.**
- ▶ **Mathematical, Computational, and Computer Sciences Research.—**
 - ▶ Not less than \$300,000,000 for Mathematical, Computational, and Computer Sciences Research.

ASCR's FY2023 House Markup (cont.)

- ▶ Not less than \$15,000,000 and up to \$45,000,000 for the development of **advanced memory technologies** to advance artificial intelligence and analytics for science applications by a **U.S.-based manufacturer of memory systems and memory semantic storage**.
- ▶ The Committee supports the **Center for Advanced Mathematics for Energy Research Applications (CAMERA)** encourages the Department to support the creation of a crosscutting research program that leverages applied math, computer science and computational science to deliver artificial intelligence research, development, and deployment to increase the scientific productivity of the user facilities.
- ▶ The Department is encouraged to **explore the viability of photonic quantum computing**, in coordination with other federal agencies. The Department is encouraged to **consider mechanisms to provide access to ion trap quantum computing resources**, particularly with the ability to integrate with existing high-performance computing resources. The Department is **directed to provide to the Committee not later than 120 days after enactment of this Act a briefing on the Department's recent actions and future plans related to photonic quantum computing and ion trap quantum computing**.

FY2023 House Markup –Other Guidance

- ▶ **HBCU/MSI Engagement.**—The recommendation provides not less than \$60,000,000, including through the Reaching a New Energy Sciences Workforce (RENEW) and Funding for Accelerated, Inclusive Research (FAIR) programs,
- ▶ **Energy Earthshots.**—provides up to \$100,000,000 for Energy Earthshots, **including up to \$25,000,000 from Advanced Scientific Computing Research**, up to \$50,000,000 from Basic Energy Sciences, and up to \$25,000,000 from Biological and Environmental Research.
- ▶ **Facility Operations.**—The Committee is disappointed with the Department’s lack of support for robust user facility operations in the budget request. ...The Department is directed to prioritize the stewardship of the user facilities in fiscal year 2023 and in future budget requests.
- ▶ **Established Program to Stimulate Competitive Research.**—The recommendation provides not less than \$35,000,000 across the Office of Science programs for the Established Program to Stimulate Competitive Research.