View From Germantown

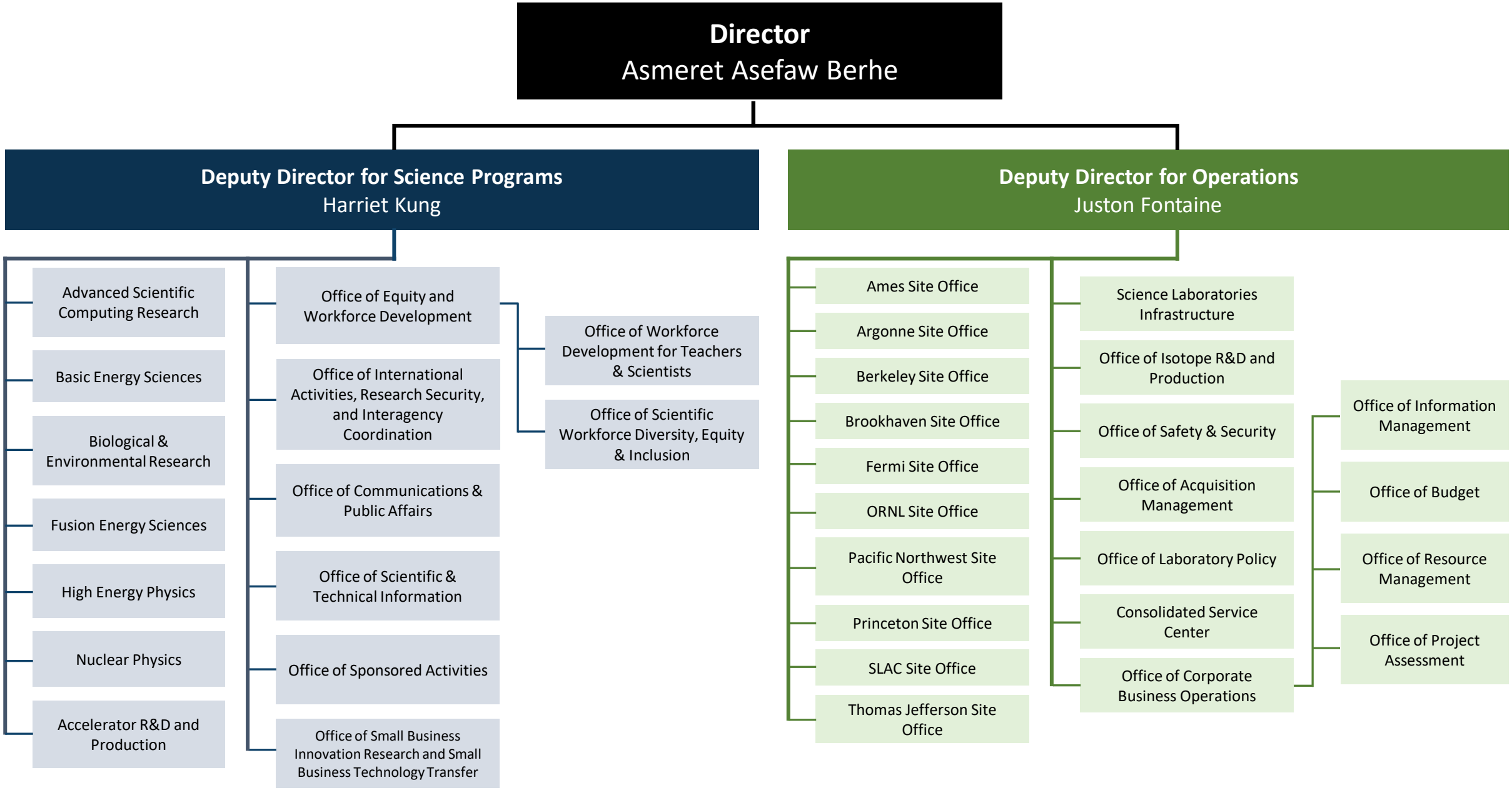
Advanced Scientific Computing Research Update

Dr. Ceren Susut

Acting Associate Director, Advanced Scientific Computing Research

June 12, 2023

SC Realignment


Director
Asmeret Asefaw Berhe
Deputy Director for Science Programs
Harriet Kung
Advanced Scientific Computing Research
Basic Energy Sciences
Biological & Environmental Research
Fusion Energy Sciences
High Energy Physics
Nuclear Physics
Accelerator R&D and Production
Office of Equity and Workforce Development
Office of Workforce Development for Teachers & Scientists
Office of Scientific Workforce Diversity, Equity & Inclusion
Office of International Activities, Research Security, and Interagency Coordination
Office of Communications & Public Affairs
Office of Scientific & Technical Information
Office of Sponsored Activities
Office of Small Business Innovation Research and Small Business Technology Transfer
Deputy Director for Operations
Juston Fontaine
Ames Site Office
Argonne Site Office
Berkeley Site Office
Brookhaven Site Office
Fermi Site Office
ORNL Site Office
Pacific Northwest Site Office
Princeton Site Office
SLAC Site Office
Thomas Jefferson Site Office
Science Laboratories Infrastructure
Office of Isotope R&D and Production
Office of Safety & Security
Office of Acquisition Management
Office of Laboratory Policy
Consolidated Service Center
Office of Corporate Business Operations
Office of Information Management
Office of Budget
Office of Resource Management
Office of Project Assessment

ASCR Personnel Changes

New Adventures for Some Members

Barb Helland
Associate Director, Retired in January

Rich Carlson
Program Manager, Retired in December

Tameka Morgan
Administrative Assistant, NOAA since January

Angie Thevenot
Program Support Specialist, BES since May

Hal Finkel
Program Manager, Acting Research Division Director since February

Robinson Pino
Program Manager, Detail at CHIPS since October

Welcome New Members

Kalyan Perumalla is a Program Manager in the Research Division. Previously, he was a Distinguished Research Staff Member at ORNL in the computing research divisions. He has a Ph.D. in Computer Science.

David Rabson joins as a Program Manager in the Research Division. Previously was an Associate Professor of Physics at University of South Florida, where he served a term as chair. He has held visiting positions at NSF.

Ashley Predith is a Senior Technical Advisor to the Research Division. She previously was the Director of the Office of Crosscutting and Special Initiatives (XCI) in SC and has a Ph.D. in computational materials science.

Jordan Thomas is in a new role in the Facilities Division as the NERSC Program Manager. She was previously the ALCC Program Manager. Jordan was a AAAS S&T Policy Fellow and has a Ph.D. in computational oceanography.

Marco Fornari is a Program Manager and will work with the SBIR program. He was a full Professor at University of Central Michigan where he worked on high throughput calculations applied to materials for energy conversion.

Abre Valencia is the new Administrative Assistant to the ASCR Associate Director. She brings 6 years of experience and is pursuing a Master's degree in Public Administration.

ASCR FY 2024 Budget Update

ASCR FY 2024 President's Request

(dollars in thousands)

	FY 2022 Enacted	FY 2023 Enacted	FY 2024 Request	FY 2024 Request vs FY 2023 Enacted		FY 2024 Request vs FY 2022 Enacted	
Advanced Scientific Computing Research							
Applied Mathematics Research	50,858	61,035	76,188	+15,153	+24.83%	+25,330	+49.81%
Computer Sciences Research	49,963	60,667	86,017	+25,350	+41.79%	+36,054	+72.16%
Computational Partnerships	79,456	95,875	87,600	-8,275	-8.63%	+8,144	+10.25%
Advanced Computing Research	105,723	108,920	149,848	+40,928	+37.58%	+44,125	+41.74%
Energy Earthshot Research Centers	–	12,500	12,500	–	–	+12,500	–
Total, Mathematical, Computational, and Computer Sciences Research	**286,000**	**338,997**	**412,153**	**+73,156**	**+21.58%**	**+126,153**	**+44.11%**
High Performance Production Computing	120,000	132,003	142,000	+9,997	+7.57%	+22,000	+18.33%
Leadership Computing Facilities	410,000	430,000	466,607	+36,607	+8.51%	+56,607	+13.81%
High Performance Network Facilities and Testbeds	90,000	90,000	90,213	+213	+0.24%	+213	+0.24%
Total, High Performance Computing and Network Facilities	**620,000**	**652,003**	**698,820**	**+46,817**	**+7.18%**	**+78,820**	**+12.71%**
17-SC-20, SC Exascale Computing Project	**129,000**	**77,000**	**14,000**	**-63,000**	**-81.82%**	**-115,000**	**-89.15%**
Total, Advanced Scientific Computing Research	**1,035,000**	**1,068,000**	**1,125,973**	**+57,973**	**+5.43%**	**+90,973**	**+8.79%**

FY 2024 President's Request of $1,126 million is an increase of $58 million or 5.4%, above the FY 2023 Enacted Budget.

ASCR FY 2024 President's Request

ASCR Total (FY23 $1,068,000), FY24: $1,125,973)	**+$57,973**
Mathematical, Computational, and Computer Sciences Research (FY23: $338,997, FY24: $412,153)	**+$73,156**
• Applied Math: Increase supports investments in basic research that addresses specific cross-cutting applied math challenges for Energy Earthshots.	+$15,153
• Computer Science.: Increase supports investments in basic research that addresses specific cross-cutting applied math challenges for Energy Earthshots. The increase also reflects moving quantum computing research investments from Computational Partnerships.	+$25,350
• Computational Partnerships: Maintains support continued partnerships across SC – including Accelerate and FAIR and scientific discovery for cancer and biopreparedness (BRAVE). The decrease reflects moving quantum computing research funding to Computer Science.	-$8,275
• Advanced Computing Research: Increase supports new microelectronics research centers, CSGF and RENEW.	+$40,928
• Energy Earthshots Research Centers: Maintains to support for the joint efforts with BES and BER.	+$0

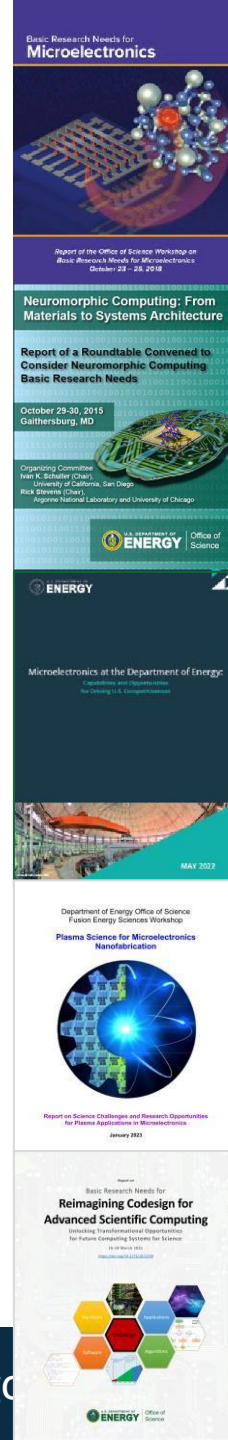
ASCR FY 2024 President's Request

Exascale Computing Project (FY23: $77,000, FY24 $14,000): Decrease reflects shift to project close out and documentation.	**-$63,000**
High Performance Computing and Network Facilities (FY23 $652,003; FY24: $698,820)	**+$46,817**
• High Performance Production Computing: Increase supports site preparation and NRE activities for NERSC-10 and planning and evaluation of designs for high-performance data facility.	+$9,997
• Leadership Computing Facilities: Increase supports operation and competitive allocation of both exascale systems and planning for future upgrades and vendor partnerships.	+$36,607
• High Performance Network Facilities and Testbeds: Increase supports planning activities for IRI.	+ $213

Microelectronics Science Research Centers

FY 2024 Request: $60M across SC ($25M in ASCR)

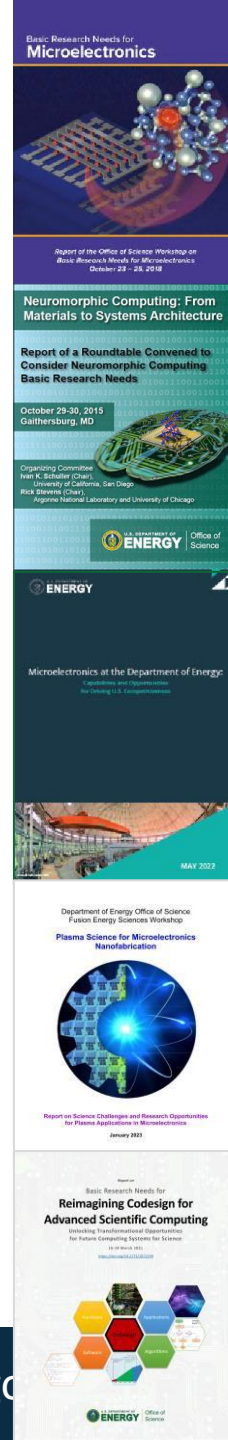
- CHIPS and Science Act (Section 10731, Micro Act) authorizes DOE to establish a crosscutting program of RD&D in microelectronics relevant to DOE missions, including establishing up to four new SC **Microelectronics Science Research Centers** to perform mission-driven research to address foundational challenges in the design, development, characterization, prototyping, demonstration, and fabrication of microelectronics.
  - Complements existing SC microelectronics awards
- SC-wide Centers would focus on fundamental science and early-stage research, complementing the investments already made through the CHIPS Act, most relevantly:
  - Department of Commerce National Semiconductor Technology Center: Focused on later-stage prototyping and applied RD&D; requires external basic research for success
  - Department of Defense (DOD) Microelectronics Commons: Focused on capabilities required for DOD; unlikely to address most DOE mission areas
- Centers would leverage the broad infrastructure and expertise at the DOE National Labs as well as in academia and industry.



Microelectronics Science Research Centers

FY 2024 Request: $60M across SC ($25M in ASCR)

- Potential areas of emphasis include:
  - Accelerated discovery and development of new microelectronics science and technology
  - Advanced experimental and computational capabilities, including materials science, chemistry, plasma science, artificial intelligence, and multiscale co-design
  - Innovative methods for circuits, architectures, systems, modeling, and synthesis
  - Sustainable and energy-efficient microelectronics devices, including logic, memory, and sensors/detectors
  - Testbeds for prototyping platforms for validation/verification of new concepts; Prototyping of novel devices to facilitate lab-to-fab transition
    - Development of advanced cybersecurity capabilities for computing architectures



ASCR FY 2023 Update

FY2023 ASCR Solicitations

Title	Max DOE Funding	Announcement Release	Proposals Due
Distributed Resilient Systems	$45,000,000	12/14/2022	3/30/2023
Funding for Accelerated, Inclusive Research (FAIR)	$35,000,000 (*)	12/15/2022	4/11/2023
Reaching A New Energy Sciences Workforce (RENEW)	$10,000,000	1/9/2023	4/18/2023
Energy Earthshot Research Centers	$200,000,000 (*)	1/18/2023	5/31/2023
Scientific Machine Learning for Complex Systems	$16,000,000	1/24/2023	4/19/2023
Biopreparedness Research Virtual Environment (BRaVE)	$105,000,000 (*)	1/24/2023	5/9/2023
(*) Total funds for includes funding from ASCR and partnering programs			

FY2023 ASCR Solicitations (Continued)

Title	Max DOE Funding	Announcement Release	Proposals Due
Exploratory Research for Extreme-Scale Science (EXPRESS)	$10,000,000	2/2/2023	4/19/2023
• Modeling Future Supercomputing Systems			
• Programming Techniques for Computational Physical Systems			
• Quantum Algorithms across Models			
Accelerate Innovations in Emerging Technologies (ACCELERATE)	$80,000,000 (*)	2/16/2023	6/7/2023
(*) Total funds for includes funding from ASCR and partnering programs			

FY2023 ASCR Solicitations (Continued)

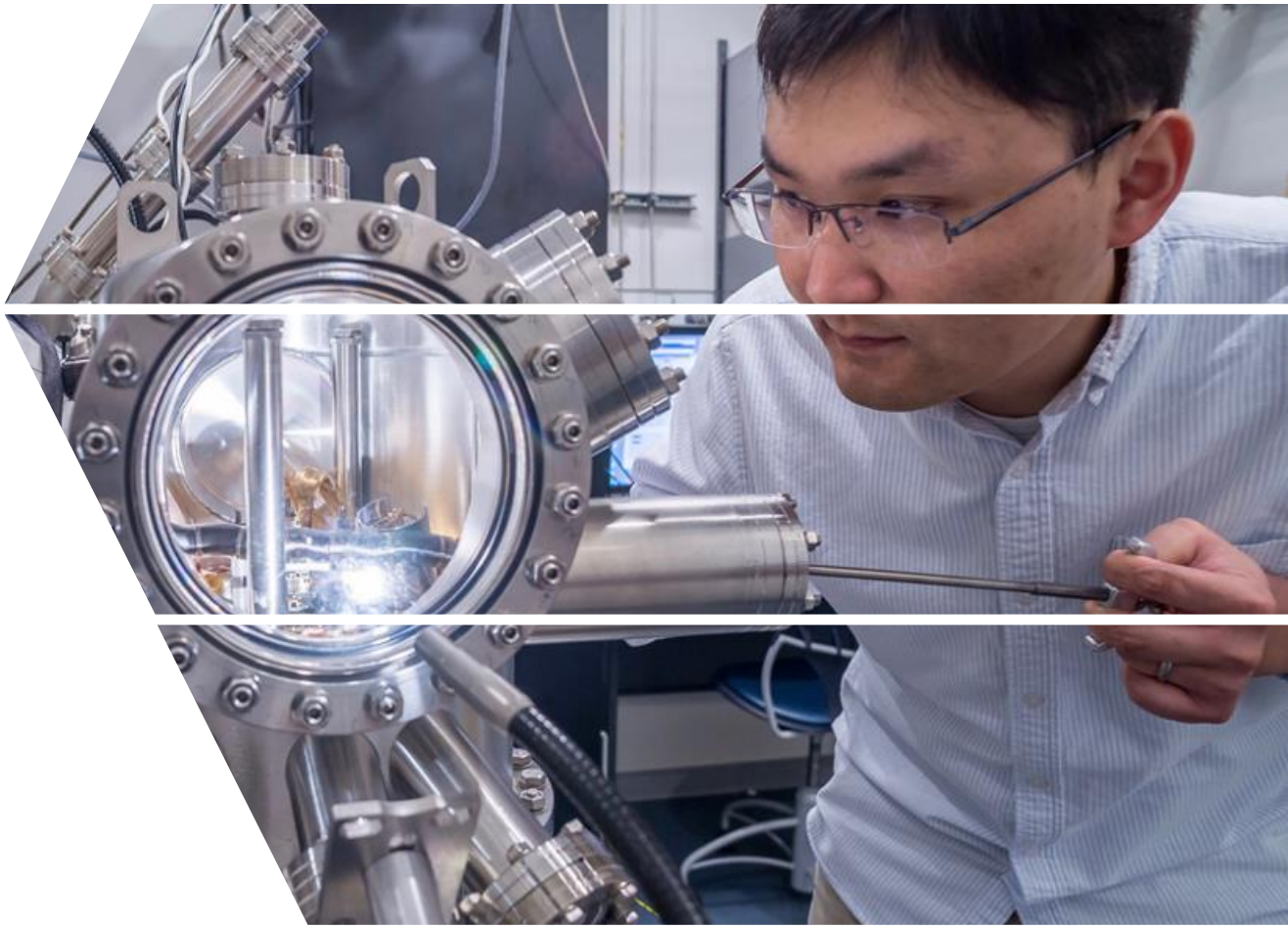
Title	Max DOE Funding	Announcement Release	Proposals Due
Quantum Testbed Pathfinder	$12,000,000	3/1/2023	5/3/2023
Scientific Discovery Through Advanced Computing (SciDAC) - FES Partnerships	$120,000,000 (*)	3/8/2023	5/19/2023
High Performance Data Facility	$300,000,000	3/10/2023	5/5/2023
Science Foundations for Energy Earthshots	$150,000,000 (*)	3/21/2023	6/21/2023
Advanced Scientific Computing Research for DOE User Facilities	$27,000,000 (*)	4/3/2023	6/7/2023
Scientific Enablers of Scalable Quantum Communications	$24,000,000	4/18/2023	6/5/2023
(*) Total funds for includes funding from ASCR and partnering programs			

“New” Solicitations

- **High Performance Data Facility (HPDF):** National Laboratory Funding Announcement – will support a new scientific user facility specializing in advanced infrastructure for data-intensive science. HPDF is envisioned as foundational to advancing DOE’s integrated research infrastructure and a broad spectrum of data-intensive research and will be designed to dynamically configure computation, network resources, and storage to access data at rest or in motion, supporting the use of well-curated datasets as well as near real-time analysis on streamed data directly from experiments or instruments.
- **Advanced Scientific Computing Research for DOE User Facilities:** National Laboratory Funding Announcement – will support development of advanced algorithms and software stacks for new and emerging techniques at DOE light and neutron user facilities to enable on-the-fly data analysis and autonomous experimentation. (Supported by ASCR and BES)

Promoting Inclusive and Equitable Research (PIER) Plan

- All new and renewal proposals are required to submit a PIER Plan
- The complexity and detail of the plan is expected to increase with the size of the research team
- The PIER Plan will be evaluated under a new merit review criterion as part of the peer review process



ASCR Software Sustainability

- *Key question*: How should ASCR best support continuing software-technology development and community vibrancy in the exascale science era, across next-generation HPC systems, and advanced scientific computing broadly?
  - Researchers often develop software needed for their research, but research funding is often short term and does not support maintaining and improving the software for use by other researchers, other agencies, and industry.
  - The Exascale Computing Project (ECP) has developed and implemented best practices for software sustainability for the past seven years. However, ECP will wrap up successfully during FY 2024.
- What resources and stewardship models are needed by the community? The community identified needs and responded to ASCR's Request for Information in October 2021:
  - Training on software development and use and on best practices for community development/management
  - Community outreach and networking, legal and administrative support, application engagement and support, and workforce support
  - Infrastructure for common development needs
  - Curation and governance processes and maintaining situational awareness
  - Shared engineering resources and project support (including the incorporation of new capabilities)
  - For additional information, see https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202203/ASCAC_202203_Finkel-RFI-Codesign-PDES.pdf

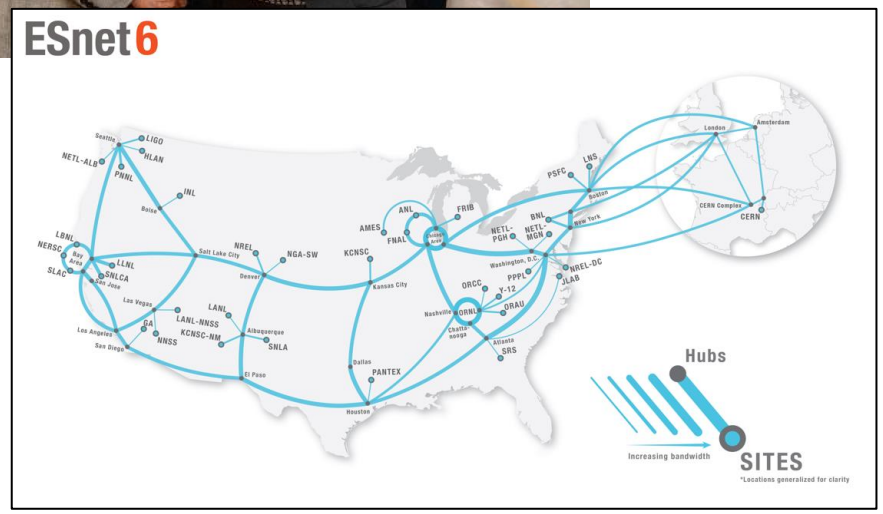
ASCR Software Sustainability – Seed Collaborations

- 6 collaborations were selected after peer review from proposals submitted under the DOE SC Open Call and submitted by DOE National Laboratories. Total funding, from ASCR Advanced Computing Technology and Facilities Divisions, is $720 thousand for one year.
- Collaborations are now engaging with the HPC and scientific-software communities to gather requirements, build coalitions, and plan for the future.
- ***To the ASCR community***: please reach out to the collaborations that might be relevant to your future activities, and where synergies may exist, help the collaborations understand your requirements, and work to understand how the activities that the collaboration envisions might help meet your future needs.

ASCR Facilities Updates

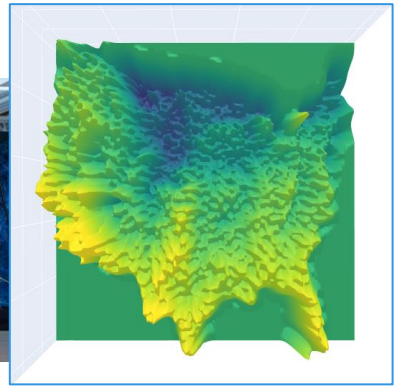
DOE honored ESnet for project management excellence: ESnet6 was completed under budget and two years ahead of schedule.

ESnet6 Project Director Kate Mace received the award on behalf of the project team from OPA Director Kurt Fisher in April.



In May, we bid farewell to the NERSC-8 Cori system, the longest operating supercomputer in NERSC's 49-year history.

The NERSC-9 Perlmutter system is in final shakeout. Early science has been highly productive. Researchers recently demonstrated a new approach to spare matric Gaussian processes leveraging a GPU-enabled 30X speedup compared to Cori.



NERSC recently released the draft Technical Specifications for NERSC-10 and is preparing to seek Critical Decision 1 in early 2024.

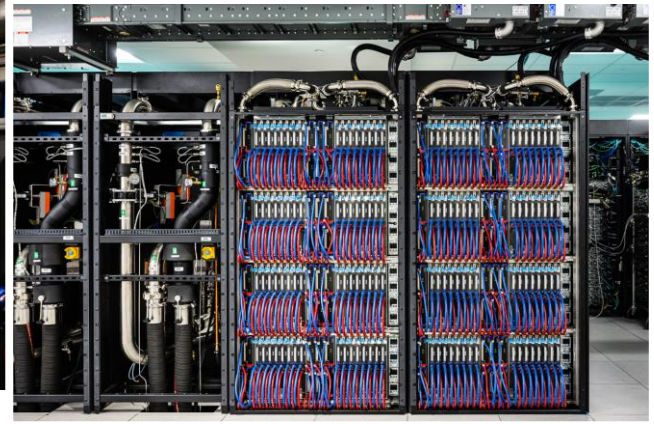
ASCR Facilities Updates

OLCF's Frontier system remains #1 on the Top500. Its Linpack gain of 92 PF is equivalent to the #7 system on the list. Its HPL-MxP performance increased to 9.95 EF.

In April <u>all</u> allocation programs were enabled on Frontier: INCITE, ECP, ALCC (small), and Director's Discretionary with more than 8M node-hours delivered so far.

Highlight: PNNL's Exascale Grid Optimization (ExaGO) application demonstrated whole-grid model runs in under 20 minutes, which is meaningful for real-world grid operations decision timeframes.

The ALCF Aurora project recently achieved a major milestone. Today at 3:00pm ET, ALCF-3 Project Director Susan Coghlan will provide an overview of Aurora.



ALCF deployed Aurora's Sunspot Test and Development system and early science runs are going well. Over 180 researchers from 20+ application teams have used the system.

In May, ALCF expanded its AI Testbed program, adding a new Graphcore system along with upgraded Cerebras and SambaNova machines.

Notable Reviews: Many Thanks to All Teams

- **National QIS Research Centers:** Mid-Term progress review of the 5 Centers held in February-March. 10 reviewers provided feedback on strengths, concerns and constructive suggestions on: Technical Areas, S&T Innovation Chain, Ecosystem Stewardship, Management Structure, Instrumentation and Facilities. No major issues identified.
- **Exascale Computing Project Independent Project Review:** Held in May. 10 reviewers evaluated the project based on the following charge questions: 1) Is the project making adequate progress to address the recommendations and comments from the March 2022 Independent Project Review? 2) Is the project on track to meet its threshold KPPs? 3) Is the ECP adequately prepared for project close-out? 4) Are risks adequately identified and managed with appropriate responses? Is there adequate contingency to successfully complete the project? 5) Is the overall project being properly managed? No issues identified.

Celebrating World Quantum Day

Public webinar in partnership with BES that showcased the broad range of user facilities and other infrastructure capabilities that work in QIS.

April 14, 2023

Dr. Asmeret Asefaw Berhe
Director, Office of Science
Welcome Remarks

Dr. Pranav Gokhale
Infleqtion's VP of Quantum Software

Dr. Kathleen Hamilton
Research scientist at ORNL

Dr. Suji Park
Scientist at Center for Functional Nanomaterials, BNL

Professor Zhi-Xun Shen
Professor of Physics at Stanford University

Video at https://science.osti.gov/Initiatives/QIS

AI4SES Report Published

https://www.anl.gov/ai-for-science-report

Argonne NATIONAL LABORATORY

RESEARCH WORK WITH US COMMUNITY ABOUT US

READ THE REPORT

Over the past decade, fundamental changes in artificial intelligence (AI) have delivered dramatic insights across a wide breadth of U.S. Department of Energy (DOE) mission space. AI is helping to augment and improve scientific and engineering workflows in national security, the Office of Science, and DOE's applied energy programs. The progress and potential for AI in DOE science was captured in the 2020 "AI for Science" report. In the short interim, the scale and scope of AI have accelerated, revealing new, emergent properties that yield insights that go beyond enabling opportunities to being potentially transformative in the way that scientific problems are posed and solved. These AI advances also highlight the crucial importance of responsible development of AI, focusing on challenges relating to AI *technology* (e.g., explainability, validation, security and privacy), *implementation* (e.g., transparency, safety engineering, ethics), and *application* (e.g., AI-Human interactions, education, and employment impacts).

SHARE

RELATED ORGANIZATIONS

Computing, Environment and Life Sciences

RELATED REFERENCES

AI for Science Report 2020

Argonne, Oak Ridge, and Berkeley national laboratories hosted four AI for Science town halls attended by more than a thousand scientists and engineers. Following the town halls, an AI for Science Report was compiled.

READ MORE

ASCR Basic Research Needs in Quantum Computing and Networking - July 11-13, 2023

https://www.orau.gov/ASCR-BRN-Quantum

- Workshop will identify priority research directions in quantum computing and networking research.
- Topics covered will include:
  - Applications
  - Computing and programming models
  - Algorithms
  - Compilation
  - Error correction and mitigation
  - Codesign and integration across the quantum computing and networking stacks
  - For additional information, see the pre-workshop document posted on the workshop website.

- Registration for virtual plenary-session attendance is currently open – visit the workshop website to register.

Deb Agarwal Retirement from LBNL

Deb is an internationally recognized expert in data science. She has been instrumental in designing and developing data systems for critical scientific problems in support of DOE's missions since she joined Berkeley Lab in 1994.

- Berkeley Lab's Director's Exceptional Achievement Award in 2015
- Top 25 Women of the Web Award in 2000
- Honorary doctorate in 2020

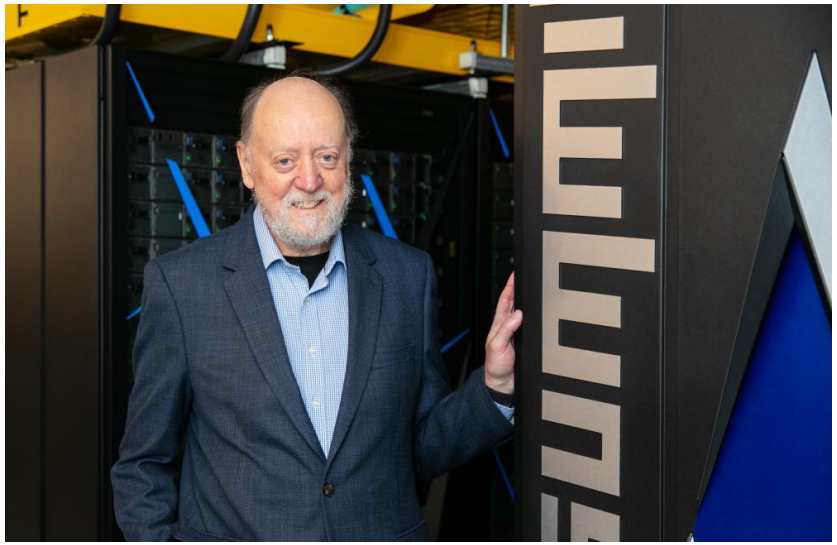
BERKELEY LAB

Jack Dongarra Elected to National Academy of Sciences

ASCAC member Jack Dongarra has been elected to NAS in recognition of his distinguished and continuing achievements in original research.

Jack previously won the 2021 ACM A.M. Turing Award for innovative contributions to numerical algorithms and libraries that enabled high-performance computational software to keep pace with exponential hardware improvements for over four decades.

- Distinguished Research Staff, Oak Ridge National Laboratory
- Turing Fellow, University of Manchester
- University Distinguished Professor (emeritus), University of Tennessee, Knoxville



https://www.ornl.gov/news/dongarra-elected-national-academy-sciences

Credit: Genevieve Martin

ANL’s Rusty Lusk honored with community symposium

Friends, colleagues and collaborators of Ewing “Rusty” Lusk came together to celebrate his life and career and explore the future of computing at a symposium held April 13-14, 2023 at ANL.

Jack Dongarra speaks at the symposium.

Valerie Taylor elected a fellow of AAAS

ASCAC member Valerie Taylor has been named AAAS fellow for her contributions to the performance analysis and modeling of high-performance scientific applications and leadership with broadening participation in computing.

► Director of the MCS Division and Argonne Distinguished Fellow, Argonne National Laboratory
► Professor and Department Head of Computer Science and Engineering, Texas A&M University
► Faculty member in the Electrical Engineering and Computer Science Department at Northwestern University

Some ASCAC Agenda Details

- OFFICE OF SCIENCE WELCOME – *Asmeret Asefaw Berhe, Director of the Office of Science*
- ECP UPDATE – *Lori Diachin, ECP Director*
- UPDATE ON AURORA – *Susan Coghlan, Argonne National Laboratory*
- TOWARD AN INTEGRATED RESEARCH INFRASTRUCTURE – *Ben Brown, ASCR*
- AI FOR SCIENCE, ENERGY AND SECURITY WORKSHOPS AND REPORT – *Rick Stevens, Argonne National Laboratory*
- *NQIAC REPORT – Charlie Tahan, NQCO*
- SUBCOMMITTEE REPORTS
  - DOE-NCI COLLABORATIONS – *Tony Hey, ASCAC*
  - INTERNATIONAL BENCHMARKING – *Jack Dongarra, ASCAC*

Back-Up

ASCR Software Sustainability – Seed Collaborations

Principal Investigator	Title	Lead Organization	Collaborating Organizations
Dubey, Anshu	COLABS: Collaboration of ORNL, LBNL, and ANL for Better Software	Argonne National Laboratory	Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory
Ferreira da Silva, Rafael	Center for Sustaining Workflows and Application Services	Oak Ridge National Laboratory	Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory
Heroux, Michael	Toward a Post-ECP Software-Sustainability Organization (PESO)	Sandia National Laboratories	Argonne National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Sandia National Laboratories, University of Oregon
Jones, Terry	STEP: Sustainable Tools Ecosystem Project	Oak Ridge National Laboratory	Advanced Micro Devices, Inc.; Ames National Laboratory; Argonne National Laboratory; Hewlett Packard Enterprise; Intel Corporation; International Business Machines Corporation; Lawrence Berkeley National Laboratory; Lawrence Livermore National Laboratory; Los Alamos National Laboratory; Northeastern University; Pacific Northwest National Laboratory; Rice University; Sandia National Laboratories; University of Oregon; University of Tennessee; University of Wisconsin
(Continued on the next slide)			

ASCR Software Sustainability – Seed Collaborations

Principal Investigator	Title	Lead Organization	Collaborating Organizations
(Continued from the previous slide)			
Teranishi, Keita	S4PST: Sustainability for Node Level Programming Systems and Tools	Oak Ridge National Laboratory	Argonne National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Louisiana State University, Massachusetts Institute of Technology, University of Delaware, University of Oregon
Watson, Gregory	Open Scientific Software Foundation	Oak Ridge National Laboratory	Eclipse.org Foundation, Inc.; The HDF Group; Kitware, Inc.; Sandia National Laboratories; University of Illinois Urbana-Champaign