Advanced Scientific Computing Research Update

Ceren Susut, PhD

Associate Director of Science

for Advanced Scientific Computing Research
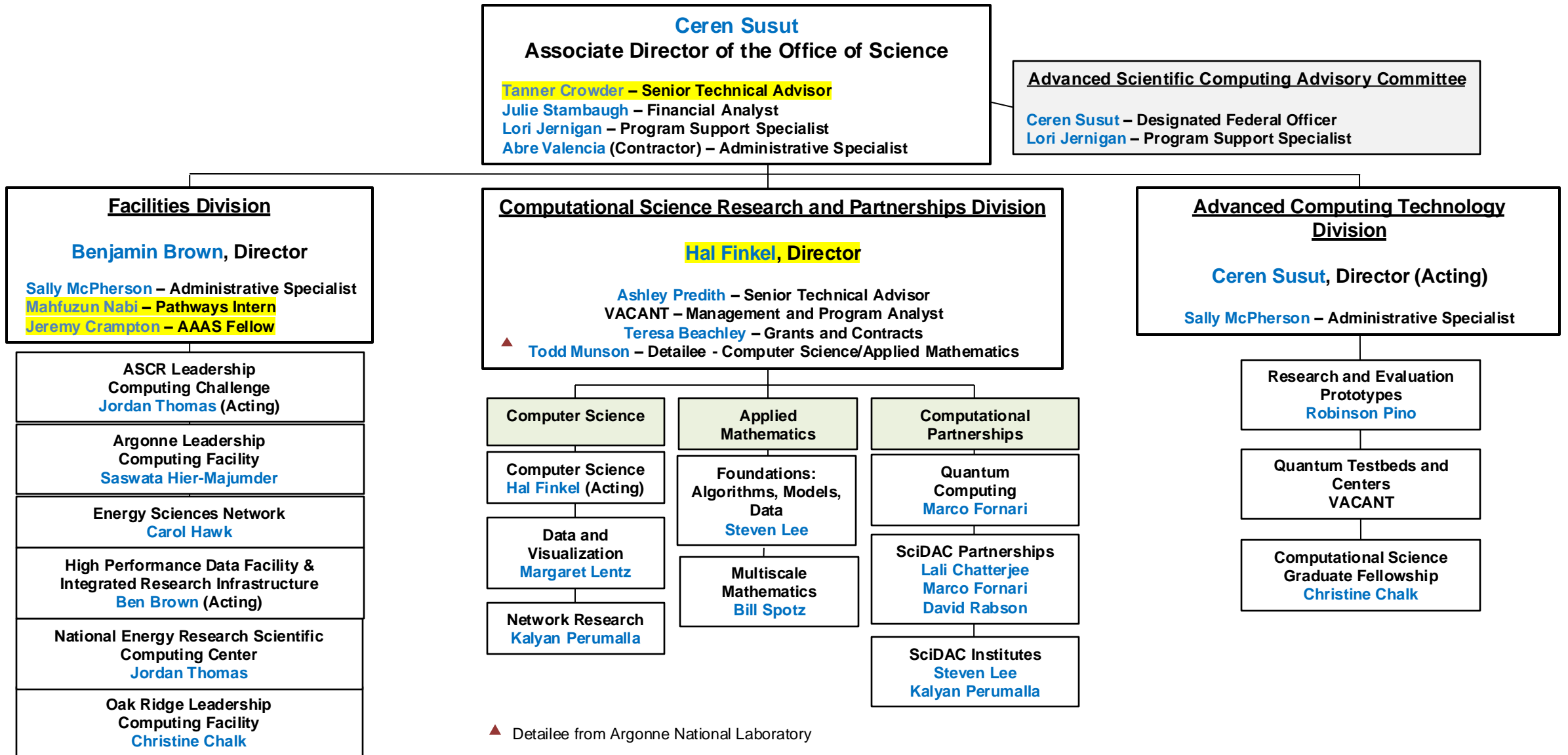
U.S. DEPARTMENT OF ENERGY | Office of Science

U.S. Department of Energy Office of Science
Office of

ADVANCED SCIENTIFIC COMPUTING RESEARCH

Functional Organization Chart

Ceren Susut
Associate Director of the Office of Science

Tanner Crowder **– Senior Technical Advisor**
Julie Stambaugh **– Financial Analyst**
Lori Jernigan **– Program Support Specialist**
Abre Valencia (Contractor) **– Administrative Specialist**

Advanced Scientific Computing Advisory Committee

Ceren Susut **– Designated Federal Officer**
Lori Jernigan **– Program Support Specialist**

Facilities Division

Benjamin Brown, Director

Sally McPherson **– Administrative Specialist**
Mahfuzun Nabi **– Pathways Intern**
Jeremy Crampton **– AAAS Fellow**

ASCR Leadership Computing Challenge
Jordan Thomas (Acting)

Argonne Leadership Computing Facility
Saswata Hier-Majumder

Energy Sciences Network
Carol Hawk

High Performance Data Facility & Integrated Research Infrastructure
Ben Brown (Acting)

National Energy Research Scientific Computing Center
Jordan Thomas

Oak Ridge Leadership Computing Facility
Christine Chalk

Computational Science Research and Partnerships Division

Hal Finkel, Director

Ashley Predith **– Senior Technical Advisor**
VACANT **– Management and Program Analyst**
Teresa Beachley **– Grants and Contracts**
▲ Todd Munson **– Detailee - Computer Science/Applied Mathematics**

Computer Science

Computer Science
Hal Finkel (Acting)

Data and Visualization
Margaret Lentz

Network Research
Kalyan Perumalla

Applied Mathematics

Foundations: Algorithms, Models, Data
Steven Lee

Multiscale Mathematics
Bill Spotz

Computational Partnerships

Quantum Computing
Marco Fornari

SciDAC Partnerships
Lali Chatterjee
Marco Fornari
David Rabson

SciDAC Institutes
Steven Lee
Kalyan Perumalla

Advanced Computing Technology Division

Ceren Susut, Director (Acting)

Sally McPherson **– Administrative Specialist**

Research and Evaluation Prototypes
Robinson Pino

Quantum Testbeds and Centers
VACANT

Computational Science Graduate Fellowship
Christine Chalk

▲ Detailee from Argonne National Laboratory

Dr. Hal Finkel

Computational Science Research & Partnerships Division Director

Hal joined ASCR in October 2020 as a Program Manager in the CSRP Division for computer science research and in February 2023, he was detailed to serve as the Acting Division Director of the CSRP Division.

Prior to joining ASCR, Hal spent nearly a decade at the Argonne National Laboratory as a physicist and computational scientist at Argonne's Leadership Computing Facility (ALCF). Hal built and led a team at Argonne focused on advancing the computer science of compiler technology and programming languages. The team contributed significantly to the efforts of the Exascale Computing Project (ECP) in addition to exploring artificial intelligence, quantum computing, spatial architectures, and other forward-looking technologies. Hal served as vice chair of the C++ standards committee for five years and served on the board of directors of the LLVM Foundation, a nonprofit with a mission to support education and to increase diversity in compilers research.

Hal holds a Ph.D. in Physics from Yale University, where he focused on early-universe cosmology, and a Bachelor of Science, Physics from Drexel University.

Dr. Tanner Crowder

Senior Technical Advisor

Tanner joined DOE in September 2024 as Senior Technical Advisor to ASCR.

Prior to joining ASCR, Tanner spent over 15 years as a research mathematician at the Naval Research Laboratory, where he served as PI on several projects advancing quantum computing, sensing, and communications. For the last 3 years, Tanner has been detailed National Quantum Coordination Office at the White House Office of Science and Technology Policy. There he serves as a Senior Policy Advisor and has led activities around the economic and national security implications of QIS and access to quantum-related R&D, as well as industrial engagement.

Tanner earned a B.S. in Mathematics and Physics from The College of William and Mary and a Ph.D. in Mathematics from Howard University.

The Facilities Division welcomes two new members

Mahfuzun Nabi is a new federal Pathways intern in the Facilities Division with an appointment through December 2024.

Mahfuzun recently completed his M.S. degree in physics from California State University, Long Beach, with a thesis on Angle-Resolved Photoemission Spectroscopy on Dirac Semimetals; he has experience as a user of the Advanced Light Source at LBNL. He obtained his bachelors in physics with a minor in mathematics from the University of California at Los Angeles in 2022.

He will enter the physics Ph.D. program at the University of Southern California in Spring 2025.

Dr. Jeremy Crampton is a new AAAS Science & Technology Policy Fellow in the Facilities Division with an appointment through August 2025.

Jeremy comes to ASCR with three decades of experience in academia at George Mason University, Georgia State, and the University of Kentucky, and Newcastle University (UK) as Professor of Urban Data Analysis.

He is an interdisciplinary social scientist and geographer, with research interests in spatial science, mapping, Geographic Information Science, and geospatial technologies. His research focused on the socio-political aspects of location technologies, and algorithmic governance in the areas of spatial data protection and privacy. He is an elected Fellow of the Academy of Social Sciences (UK) and a former Fellow of the Alan Turing Institute.

ASCR FY 2025 Request

(dollars in thousands)

	FY 2023 Enacted	FY 2024 Enacted	FY 2025 Request	FY 2025 Request vs FY 2024 Enacted		FY 2025 Request vs FY 2023 Enacted	
Advanced Scientific Computing Research							
Applied Mathematics Research	61,035	52,182	77,565	+25,383	+48.64%	+16,530	+27.08%
Computer Sciences Research	60,667	66,718	86,736	+20,018	+30.00%	+26,069	+42.97%
Computational Partnerships	95,875	75,182	93,449	+18,267	+24.30%	-2,426	-2.53%
Advanced Computing Research	108,920	108,918	148,197	+39,279	+36.06%	+39,277	+36.06%
Energy Earthshot Research Centers	12,500	5,000	12,500	+7,500	+150.00%	–	–
Total, Mathematical, Computational, and Computer Sciences Research	**338,997**	**308,000**	**418,447**	**+110,447**	**+35.86%**	**+79,450**	**+23.44%**
High Performance Production Computing	132,003	142,000	146,500	+4,500	+3.17%	+14,497	+10.98%
Leadership Computing Facilities	430,000	474,000	475,195	+1,195	+0.25%	+45,195	+10.51%
High Performance Network Facilities and Testbeds	90,000	91,000	93,540	+2,540	+2.79%	+3,540	+3.93%
Integrated Research Infrastructure	–	–	3,000	+3,000	–	+3,000	–
Total, High Performance Computing and Network Facilities	**652,003**	**707,000**	**718,235**	**+11,235**	**+1.59%**	**+66,232**	**+10.16%**
17-SC-20, SC Exascale Computing Project	**77,000**	**–**	**–**	**–**	**–**	**-77,000**	**-100.00%**
Subtotal, Advanced Scientific Computing Research	**1,068,000**	**1,015,000**	**1,136,682**	**+121,682**	**+11.99%**	**+68,682**	**+6.43%**
24-SC-20 High Performance Data Facility	–	1,000	16,000	+15,000	+1,500.00%	+16,000	–
Subtotal, Construction	**–**	**1,000**	**16,000**	**+15,000**	**+1,500.00%**	**+16,000**	**–**
Total, Advanced Scientific Computing Research	**1,068,000**	**1,016,000**	**1,152,682**	**+136,682**	**+13.45%**	**+84,682**	**+7.93%**

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ASCR's FY2025: 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**
- $219,000,000 for the Argonne Leadership Computing Facility,
- $260,000,000 for the Oak Ridge Leadership Computing Facility
- $146,500,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory
- $93,540,000 to support necessary infrastructure up-grades and operations for ESnet
- $16,000,000 in other project costs for the High Performance Data Facility
- The Department is directed to provide to the Committee not later than 180 days after enactment of this Act a report that includes an analysis and discussion of the Department's ongoing efforts to acquire high performance and quantum computing systems, advance research in quantum error correction, and develop a strategy for expanding and integrating quantum error correction research activities within the Advanced Scientific Computing Research program.

◆ **Mathematical, Computational, and Computer Sciences Research**.—
- $330,000,000 for Mathematical, Computational, and Computer Sciences Research.
- The Committee includes up to $35,000,000 to support research to develop a new path to energy efficient computing with large, shared memory pools.

ASCR's FY2025 House Markup (cont.)

- The recommendation provides not less than $245,000,000 for quantum information science, including not less than $120,000,000 for research and $125,000,000 for the five National Quantum Information Science Research Centers (Quantum Centers).

- The Department is directed to establish a roadmap that integrates the scientific goals of each of the Quantum Centers and includes a discussion of remaining goals that are to be met by future renewals of the Quantum Centers. The Committee expects that any potential renewals or re-competitions of the Quantum Centers will come only after the creation of an executable roadmap with clear outyear funding estimates.

- The Committee supports efforts to expand quantum internet, networking, and communications testbeds.

- The Committee provides up to $15,000,000 for the Department to conduct research activities in support of the Quantum User Expansion for Science and Technology program (QUEST), as authorized in the CHIPS and Science Act, to facilitate researcher access to the nation's quantum computing hardware and cloud resources and to promote a strong user base for quantum systems development.

- The Committee includes $20,000,000 to strengthen efforts to develop testbeds on high performance computing facilities to study how to effectively interface and integrate quantum processing units with traditional high performance computing resources. The Committee expects this work to be conducted in partnership with the Quantum Centers but notes that this is a new effort, and this funding direction cannot be satisfied by ongoing activities.

- The Department is encouraged to expand its relationships with NIH, including National Institute of Mental Health (NIMH), including through strategic partnership projects, to work together more strategically to leverage the Department's research capabilities, including instrumentation, materials, modeling and simulation, and data science. The facilities and equipment funded in this Act can also support applications in many areas of biomedical research, including neuropsychiatric disorders. The Committee directs the Department to coordinate with NIH and to provide to the Committee not later than 180 days after enactment of this Act a report that identifies the various national laboratory assets within the Department's portfolio that are currently being utilized by the neuroscience research community to address research on neuropsychiatric disorders.

FY2025 House Markup –Other Guidance

- **Justice40 Initiatives –**The recommendation includes no funding for the Reaching a New Energy Sciences Workforce (RENEW) or Funding for Accelerated, Inclusive Research (FAIR) initiatives.

- **Energy Earthshots –**provides $20,000,000 for Energy Earthshots, **including $5,000,000 from Advanced Scientific Computing Research,** $10,000,000 from Basic Energy Sciences, and $5,000,000 from Biological and Environmental Research.

- **Microelectronics –**The Committee notes that the current funding approach to establish four Microelectronics Centers assumes that $120,000,000 will be provided in support of these efforts over the next three years. This strategy creates immense tension between supporting ongoing research efforts and funding new initiatives in a tight fiscal environment. The Committee expects the Office of Science to ensure that any funding awards in support of the Microelectronics Centers remain flexible to ensure smaller scale research is not lost if funding for the Centers is not available in future years. In addition, as the Committee encourages

- **Established Program to Stimulate Competitive Research** –The recommendation provides not less than $35,000,000 across the Office of Science programs.

- **Artificial Intelligence (AI)**–The Committee commends the Department for its announced strategy to adopt and implement AI) in a scalable, secure, and interoperable manner. To achieve its AI goals, the Department is encouraged to consider utilizing a non-proprietary private AI architecture that allows the Department to develop and deploy Large Language Models (LLMs) and other AI models while securely maintaining control and privacy of the Department's data, models, and algorithms, with integrated security and management, on existing private and hybrid cloud technology platforms.

ASCR's FY2025: Senate Markup

▲ 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 deployable quantum computers and artificial intelligence. The Committee commends the Department of Energy and its Exascale Computing Initiative for helping the U.S. stay at the forefront of supercomputing technologies. The Committee encourages the Department to build on this model of success with a new multiyear program, leveraging public private partnerships, to co-design and co-develop leading edge post-exascale advanced computing technologies vital for continued U.S. world leadership in scientific discovery, national security and economic wellbeing.

▲ **High Performance Computing and Network Facilities**
- $225,000,000 for the Argonne Leadership Computing Facility
- $260,000,000 for the Oak Ridge Leadership Computing Facility
- $146,000,000 for the National Energy Research Scientific Computing Center
- $93,000,000 for ESnet
- $7,000,000 in other project costs for the High Performance Data Facility
- The Department is directed to provide to the Committee not later than 180 days after enactment of this act and prior to the obligation of any funds for the upgrade of the facilities, a briefing on a coordinated Department plan for what leadership computing facilities should accomplish post-exascale, including the computing technologies that will be included and the associated costs.

ASCR's FY2025: Senate Markup (cont.)

▲ **Mathematical, Computational, and Computer Sciences Research**.—

- Not less than $300,000,000 for Mathematical, Computational, and Computer Sciences Research

- Not less than $20,000,000 for CSGF

- Up to $35,000,000 to support research to develop a new path to energy efficient computing with large, shared memory pools.

- Within funding for ASCR, funding is recommended for the development of advanced memory technologies from 100s of Terabytes [TB] to Petabytes [PB] to advance artificial intelligence and analytics for science applications of very large-scale memory systems and memory semantic storage.

- The Committee directs the Office of Science to implement a hybrid HPC/Quantum Computing Pathfinder Program at a Leadership Computing Facility [LCF]. The Committee recommends up to $15,000,000 to allow the designated LCF to acquire an on-premise quantum computer via competitive process that allow the exploration of multiple technology options in order to begin to study how to effectively interface and integrate quantum processing units [QPUs] with traditional HPC resources. Additionally, the Committee recommends up to $10,000,000 for a parallel R&D program that addresses basic research challenges in algorithms and software stack for this integration to work efficiently.

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ASCR's FY2025 Senate Markup (cont.)

- **Quantum Information Science:** Not less than $265,000,000 for quantum information science, including not less than $120,000,000 for research and $125,000,000 for the five National Quantum Information Science Research Centers.

- **Artificial Intelligence and Machine Learning:** The Committee recommends $100,000,000 to implement the Frontiers in Artificial Intelligence for Science, Security, and Technology [FASST] initiative. This work shall be coordinated with the Critical Emerging Technologies Office and the National Nuclear Security Administration. Further, the Committee recommends not less than $160,000,000 for Artificial Intelligence and Machine Learning across the Office of Science Programs. As the stewards of the leadership computing facilities, the Committee **expects Advanced Scientific Computing Research to take a lead role** in the Department's artificial intelligence and machine learning activities. The Committee appreciates the Department's focus on the development of foundational artificial intelligence and machine learning capabilities and encourages the Office of Science to apply those capabilities to the Office of Science's mission with a focus on accelerating scientific discovery in its Scientific User Facilities and large experiments…. The Committee recommends $5,000,000 for Critical and Emerging Technologies Office. The Department is directed within 120 days after enactment of this act to provide an AI/ML 10-year roadmap for achieving durable frontier AI/ML capabilities for the Department's AI missions for defense and non-defense. Further, the Committee recognizes that the Department of Energy, with its stewardship of 17 national laboratories, has the existing collective infrastructure and resources in advanced computing, data, and scientific workforce to help lead Federal research and development of AI. The Committee supports the Department expanding its efforts in AI consistent with the AI for Energy Report 2024 Report and the AI for Science, Energy, and Security Report released by the national laboratories in 2023 and requests that within 90 days after enactment of this act, the Department report to Congress details for the implementation of the Frontiers in Artificial Intelligence for Science, Security, and Technology [FASST] initiative. The Department is directed to coordinate and work its interagency partners including the NSF and the OSTP to further the goals of the NAIRR pilot.

ASCR's FY2025 Senate Markup (cont.)

- **Microelectronics**.—not less than $110,000,000 for microelectronics, to support innovation in the semiconductor manufacturing industry.

- **Accelerate Innovations in Emerging Technologies**.—The Committee encourages the Office of Science to continue to support the Accelerate Innovations in Emerging Technologies program and its critical work to de-risk revolutionary energy-efficient semiconductors used for AI, high-performance computing, and data centers.

- **HBCU/MSI Engagement.**—The Committee supports the Reaching a New Energy Sciences Workforce [RENEW] and the Funding for Accelerated, Inclusive Research [FAIR] initiatives.

- **Established Program to Stimulate Competitive Research.**— The Committee recommends $35,000,000 for EPSCoR.

- **Energy Earthshots.—**The Committee recommends up to $60,000,000 for Energy Earthshots, including up to $30,000,000 from Basic Energy Sciences, up to **$15,000,000 from Advanced Scientific Computing Research**, and up to $15,000,000 from Biological and Environmental Research.

FY 2025 Congressional Action: A closer look at the House and Senate Marks

($ in thousands)

	FY2024 Enacted	FY2025 Request	House Mark (not less than)	Senate Mark (not less than)
ASCR	**1,016,000**	**1,152,682**	**1,105,000**	**1,152,000**
ALCF	219,000	215,195	219,000	225,000 including ($15M for on prem quantum computer)
OLCF	255,000	260,000	260,000	260,000 including ($15M for on prem quantum computer)
NERSC	142,000	146,500	146,500	146,000
ESnet	91,000	93,540	93,540	93,000
Total Research	308,000	418,447	330,000 including $35M for large shared memory	>300,000 including $20M for CSGF, $35M large shared memory, $10M for QIS hybrid
HPDF	1,000	16,000	16,000	7,000

New ASCAC Charge: CSGF

Department of Energy
Office of Science
Washington, DC 20585

July 26, 2024

Professor Martin Berzins
Chair, Advanced Scientific Computing Advisory Committee
Professor of Computer of Science
Scientific Computing and Imaging Institute
72 S Central Campus Drive, Room 3750
Salt Lake City, UT 84112

Dear Professor Berzins:

Thank you for the recent Advanced Scientific Computing Adv
report on Facilities Subcommittee Recommendations. The rep
vision that will surely have a lasting effect on the Office of Ad
Computing Research.

- Does CSGF provide students with an effective and impactful program of appropriate quality and breadth?
- Is there a unique role for CSGF in the landscape of federal graduate fellowship programs?
- Is the program attracting diverse applicants and making awards to diverse cohorts?
- How can CSGF reach a broader applicant pool?
- Is the program appropriately tailored to support the computational scientist workforce needed at the DOE laboratories?
- What is the most effective governance model for the program?
- How should the CSGF evolve to ensure the best experience for students?
- Is the program appropriately supporting students at institutions historically underrepresented in the federal research landscape?

Please see Irene Qualters' presentation today.

ASCR Community News

◆ DOE/DARPA Collaboration in Quantum Benchmarking
  - DOE/DARPA MOU for establishing a framework for planning and coordinating future research, development, engineering, and test and evaluation activities related to quantum computing.

◆ Energy-Efficient, Analog and Neuromorphic Computing Workshops

◆ PI Meetings:
  - SciDAC PI meeting
  - First National QIS Research Centers PI meeting
  - Science Summit for Energy Earthshot Innovation

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Exascale Computing Project Officially Completed

ASCR will continue to push the frontiers in scientific breakthroughs and push innovations in HPC.
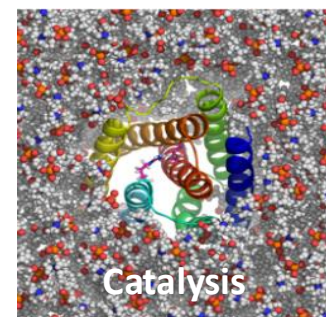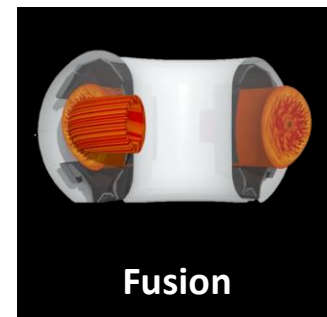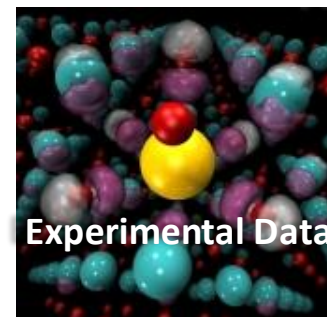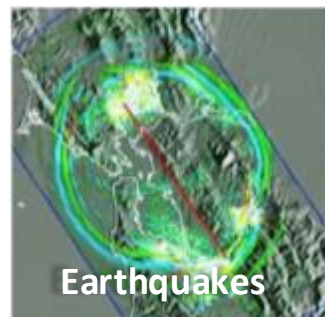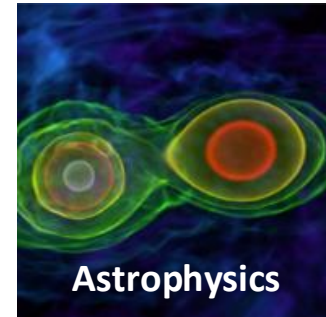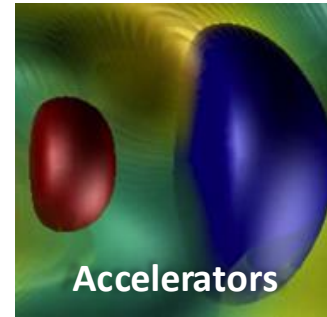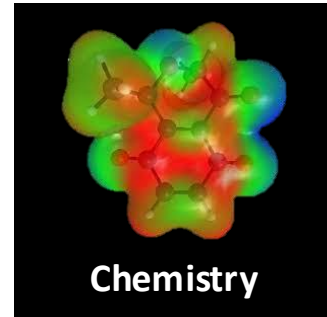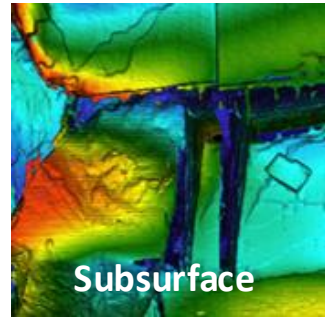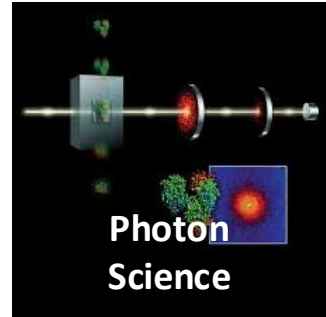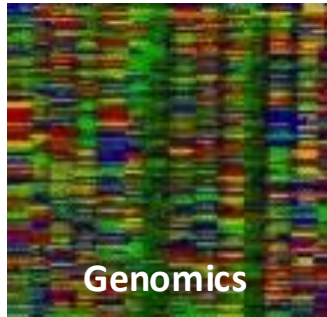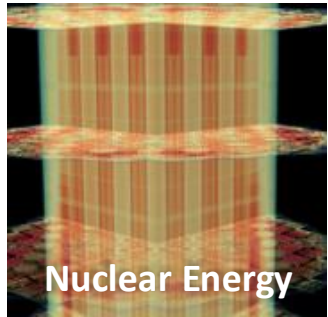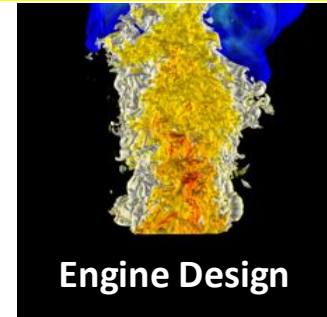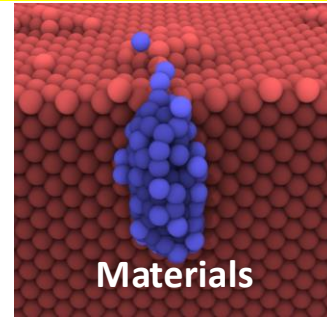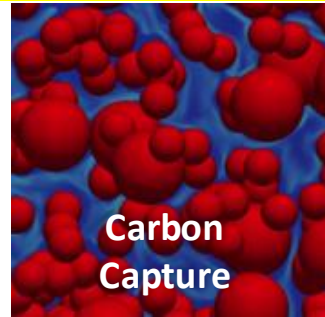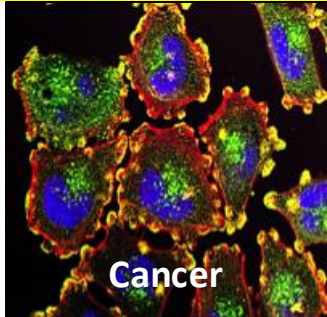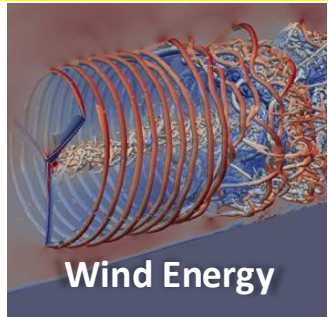
ASCR Office Hours

◆ Starting in March, ASCR started holding virtual office hours on the second Tuesday of the month, 2 PM ET

◆ Researchers, educators, and leaders within research administration from all institutional types are encouraged to join

◆ A primary goal of the virtual office hours is to broaden awareness of our programs; no prior history of funding from DOE is required to join

◆ Program managers are available to answer questions

See the ASCR website (https://science.osti.gov/ascr/officehours) for more information, including slides and recordings of past office hours.