View From Germantown
Advanced Scientific Computing Research Update

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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.

U.S. DEPARTMENT OF ENERGY | Office of Science

ASCR's FY2024: 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,
- $255,000,000 for the Oak Ridge Leadership Computing Facility
- $135,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory.
- $90,213,000 to support necessary infrastructure up-grades and operations for ESnet.
- $7,000,000 in other project costs for the High Performance Data Facility.

◆ **Mathematical, Computational, and Computer Sciences Research**.—
- $295,000,000 for Mathematical, Computational, and Computer Sciences Research.
- The Committee encourages the Department to support research to develop a new path to energy efficient computing with large, shared memory pools.

ASCR's FY2024 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.

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

- The Committee directs the Department to conduct research activities in support of the Quantum User Expansion for Science and Technology program (QUEST) as authorized in CHIPS and Science, 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 and includes up to $15,000,000 for these activities.

- The Department is directed to provide to the Committee not later than 90 days after enactment of this Act a report of near-term application developments that outlines the breakdown of research funding across the available quantum computing technologies, including gate-model, annealing, topological, photonics, trapped ion, silicon, superconducting, and other viable quantum technologies.

- 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.

U.S. DEPARTMENT OF ENERGY | Office of Science

FY2024 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 up to $20,000,000 for Energy Earthshots, **including up to $5,000,000 from Advanced Scientific Computing Research,** up to $10,000,000 from Basic Energy Sciences, and up to $5,000,000 from Biological and Environmental Research.

- **Facility Operations.—**In order to better understand the historical funding levels associated with the new optimal operations determination, the Department is directed to provide a table of user facility funding levels from the previous five fiscal years showing optimal operations using the new determination. Further, when developing any document that displays funding levels for user facility operations, the Committee expects the Department to use the same optimal operations determination for any prior, current, or future fiscal year funding levels.

- **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.

- **Mortgaging Future-Year Awards**.—The Committee remains concerned about the Department's practice of making awards dependent on funding from future years' appropriations. …The Committee expects the Department to provide information, by control point and fiscal year, on the total funding from active and closed funding opportunity announcements that are contingent on future availability of funds.

ASCR's FY2024: 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. The Committee recognizes 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. The recommendation supports efforts to maintain and improve such products in order to continuously realize the full potential of the deployed systems.

▲ **High Performance Computing and Network Facilities.— not less than**
- $219,000,000 for the Argonne Leadership Computing Facility,
- $247,607,000 for the Oak Ridge Leadership Computing Facility
- $135,000,000 for the National Energy Research Scientific Computing Center
- $91,000,000 for ESnet
- The Committee supports the President's request for the continued planning and design for the High Performance Data Facility

▲ **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.)

- **Quantum Information Science:** Not less than $255,000,000 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:** Not less than $135,000,000 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.

- **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.

- **Facility Operations.**–The Committee believes that supporting these vital user facilities should be a top priority for the Department to advance scientific discovery.

- **Microelectronics.**–the Department is encouraged to support microelectronics research and microelectronics science research centers.

- **Energy Earthshots.**–The Committee recommends up to $67,000,000 for Energy Earthshots, including up to $31,000,000 from Basic Energy Sciences, up to **$18,000,000 from Advanced Scientific Computing Research**, and up to $18,000,000 from Biological and Environmental Research.

FY 2023 Congressional Action: A closer look at the House and Senate Marks
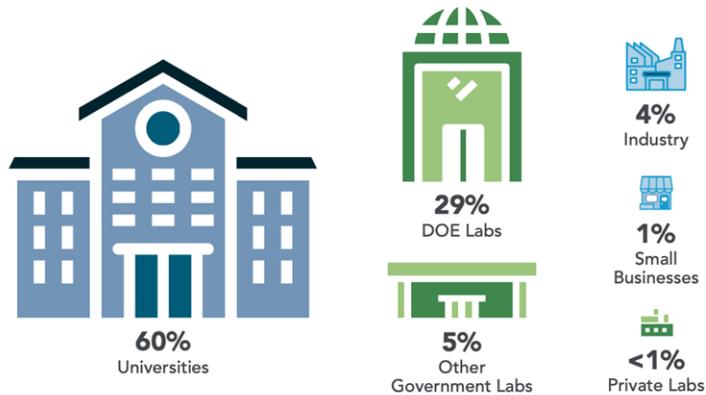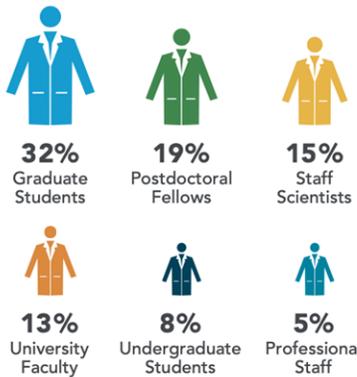
($ in thousands)

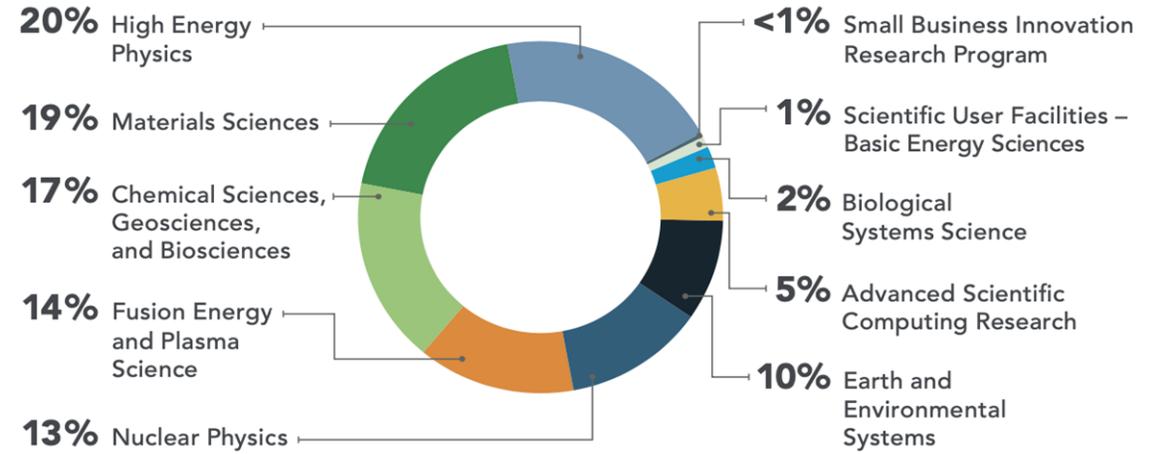|	FY2023 Enacted	FY2024 Request	House Mark (not less than)	Senate Mark (not less than)
ASCR	**1,068,000**	**1,125,973**	**1,016,213**	**1,015,973**
ALCF	175,000	219,000	219,000	219,000
OLCF	255,000	247,607	255,000	247,607
NERSC	130,000	135,000	135,000	135,000
ESnet	90,000	90,213	90,213	91,000
Total Research	338,997	412,153	295,000	>280,000 including $20M for CSGF
Exascale	77,000	14,000	14,000	14,000
High-Performance Data Facility	2,003	8,000	8,000	8,000

Perlmutter Full-System Accepted: July 2023!

- GPU nodes have been available to all NERSC users since May 2022
- Cori (previous system) was retired May 31, 2023

**~10,000 Annual Users from ~800 Institutions + National Labs**

- 32% Graduate Students
- 19% Postdoctoral Fellows
- 15% Staff Scientists
- 13% University Faculty
- 8% Undergraduate Students
- 5% Professional Staff
- 60% Universities
- 29% DOE Labs
- 5% Other Government Labs
- 4% Industry
- 1% Small Businesses
- <1% Private Labs

Breakdown of Compute Used by DOE Program

- 20% High Energy Physics
- 19% Materials Sciences
- 17% Chemical Sciences, Geosciences, and Biosciences
- 14% Fusion Energy and Plasma Science
- 13% Nuclear Physics
- <1% Small Business Innovation Research Program
- 1% Scientific User Facilities – Basic Energy Sciences
- 2% Biological Systems Science
- 5% Advanced Scientific Computing Research
- 10% Earth and Environmental Systems

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Aurora Status

◆ Full system installation completed 6/22/2023

◆ Currently in the scaling test phase

◆ Usual issues seen with serial #1 and large scale systems
  • Lustre, interconnect, and some hardware issues being worked
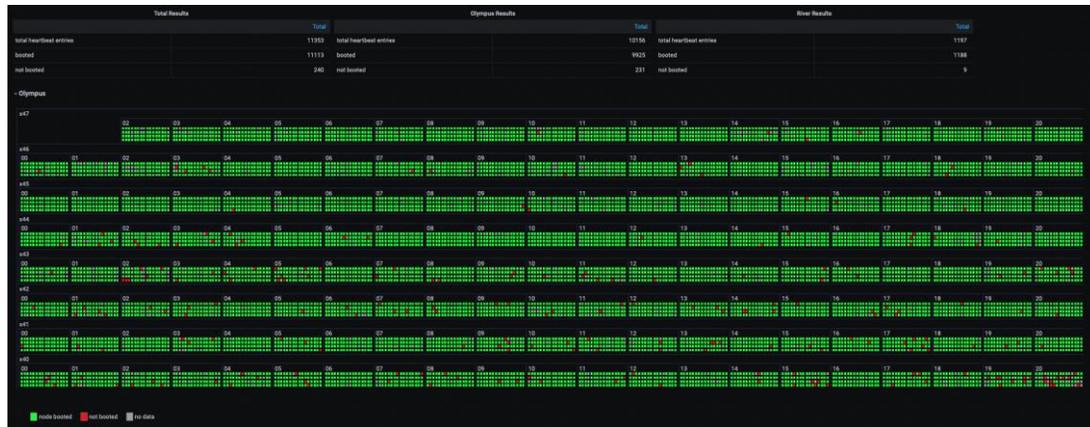
Frontier is open for science!
Delivering Exascale computing from system to ecosystem

ALL allocation programs have been enabled since April 2023

2 Gordon Bell Prize Finalists

1 Gordon Bell Climate Special Prize Finalist

To date 1,580 users & 240 projects active

GE: first-ever 3D Large Eddy Simulations at realistic flight-scale

summit PLUS

Now accepting proposals

Frontier Supercomputer
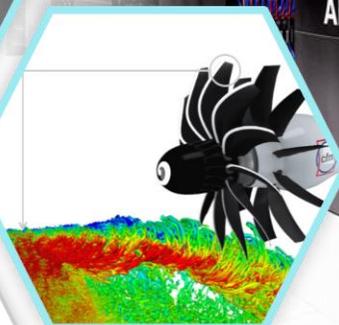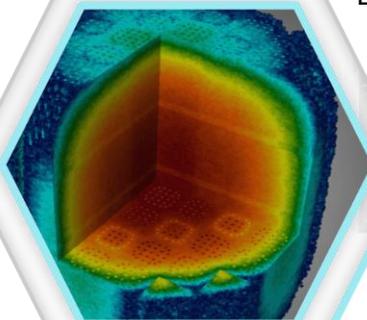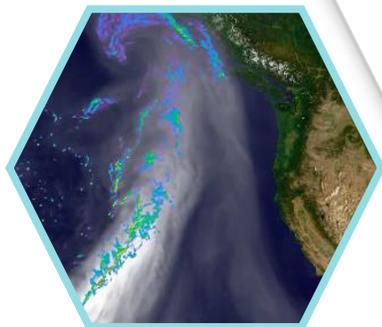
Frontier supported 3 Gordon Bell Prize Finalists in 2023

## New Alloy Discovery

Lead: University of Michigan

- Density functional theory simulation for design and discovery of new materials

- The model achieved the fastest sustained performance recorded for any materials simulation: close to 0.660 exaFLOPS using Frontier.
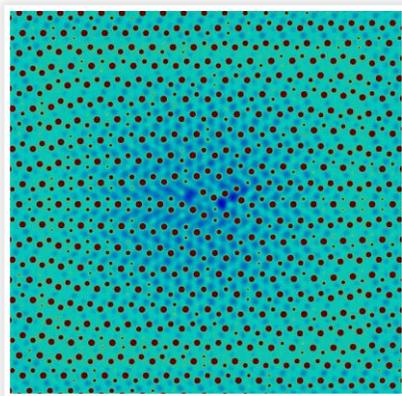
Advanced Reactor Design

Lead: Oak Ridge National Laboratory

- Multiphysics simulation of a nuclear reactor with a Monte Carlo neutron transport code coupled to a computational fluid dynamics solver

- The problem sizes and work rates they achieved on Frontier make it feasible to simulate the conditions inside a nuclear reactor with unprecedented accuracy.
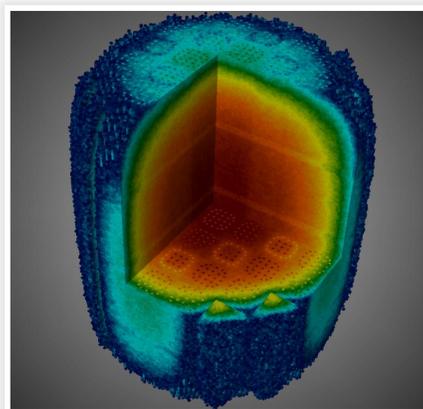
Special Prize
Atmospheric Modeling

Lead: Sandia National Labs

- Simple Cloud-Resolving E3SM Atmosphere Model, or SCREAM, a global atmospheric model

- This project broke the long-anticipated barrier of simulating more than one year per day of computation, with promise to help inform climate-change forecasts.
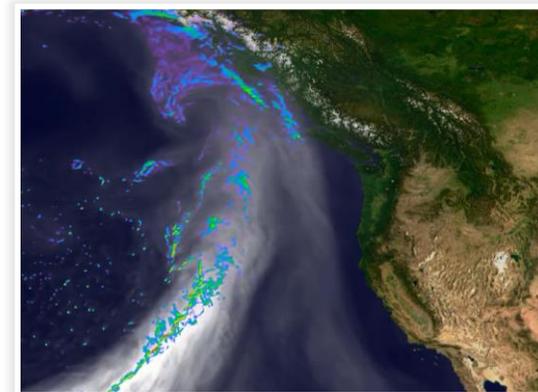
Exascale Today Enables the AI of Tomorrow

Long-term investments in applied mathematics and computer science enabled exascale.

The exascale and AI-enabled science era will lead to dramatic capabilities to predict extreme events and their impacts on the electric grid across weather and climate time scales…

MPICH
2

2005

TOP500
1

GREEN500
2

HPL-MxP
1

and will accelerate the design and deployment of clean-energy technologies to create a better future.

Frontier, #1 on the Top500, **leads the world in computational capability**, and is also **#2 in the world in energy efficiency**, and is **#1 in the world for AI capability**.

Some ASCAC Agenda Details

◆ ECP UPDATE – *Lori Diachin, ECP Director*

◆ ENERGY EXASCALE EARTH SYSTEM MODEL (E3SM) PROJECT UPDATE – *Xujing Davis, BER and Luca Bertagna, SNL*

◆ DOE-NCI COLLABORATIONS – Tony Hey, ASCAC

◆ CHIPS FOR AMERICA – *Eric K. Lin, U.S. Department of Commerce*