# The Advanced Scientific Computing Research (ASCR) User Facilities Ben Brown, Director, Facilities Division Katherine Riley, Director of Science, ALCF

https://science.osti.gov/ascr/officehours



# **Office of Science Statement of Commitment & other Guidance**

- SC Statement of Commitment SC is fully and unconditionally committed to fostering safe, diverse, equitable, inclusive, and accessible work, research, and funding environments that value mutual respect and personal integrity. <u>https://science.osti.gov/SW-DEI/SC-Statement-of-Commitment</u>
- Expectations for Professional Behaviors –SC's expectations of all participants to positively contribute to a professional, inclusive meeting that fosters a safe and welcoming environment for conducting scientific business, as well as outlines behaviors that are unacceptable and potential ramifications for unprofessional behavior. <u>https://science.osti.gov/SW-DEI/DOE-Diversity-Equity-and-Inclusion-Policies/Harassment</u>
- How to Address or Report Behaviors of Concern- Process on how and who to report issues, including the distinction between reporting on unprofessional, disrespectful, or disruptive behaviors, and behaviors that constitute a violation of Federal civil rights statutes. <u>https://science.osti.gov/SW-DEI/DOE-Diversity-Equity-and-Inclusion-Policies/How-to-Report-a-Complaint</u>
- Implicit Bias Be aware of implicit bias, understand its nature everyone has them and implicit bias if not mitigated can negatively impact the quality and inclusiveness of scientific discussions that contribute to a successful meeting. <a href="https://kirwaninstitute.osu.edu/article/understanding-implicit-bias">https://kirwaninstitute.osu.edu/article/understanding-implicit-bias</a>



# **ASCR Office Hours**

### Tuesday, July 9, 2024, at 2pm ET - Overview of the ASCR research proposal and review process.

Check the ASCR website (<u>https://science.osti.gov/ascr/</u>) for Zoom registration links and videos of prior events:

- Tuesday, May 14, 2024 Introduction to ASCR's Applied Mathematics research program. (<u>Slides</u> | <u>Video</u>)
- Tuesday, April 9, 2024 Introduction to ASCR's Computer Science research program. (<u>Slides</u> | <u>Video</u>)
- Tuesday, March 12, 2024 Introduction to ASCR and its program mission and history. (<u>Slides</u> | <u>Video</u>)



# **Open to you: ASCR Facilities Resources**

### You can seek computing allocations

- NERSC is predominantly allocated to Office of Science grantees and facility users
- The LCFs are predominantly allocated via merit review of proposals
- Quantum resources at OLCF and NERSC are allocated via merit review of proposals
- You can attend free HPC training opportunities
- You can access advice and consultation for large data transfers
- You can access open source exascale code for research applications
- You can apply for internships, postdoctoral opportunities, and staff positions



### The people of the ASCR Facilities











# **U.S. DEPARTMENT OF ENERGY** Science

### **Our Mission:**

Deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States.

Office of

More than **34,000 r**esearchers supported at more than **300** institutions and **17** DOE national laboratories

> Steward **10** of the 17 DOE national laboratories



FUNDING

More than **37,000** users of **28** Office of Science scientific user facilities

\$8.1B (FY 23 enacted)



### U.S. Department of Energy Office of Science User Facilities



U.S. DEPARTMENT OF

ENERG

Office of

Science



Lawrence Berkeley National Laboratory

Advanced Photon Source (APS)

Brookhaven National Laboratory

High Flux Isotope Reactor (HFIR)

**Spallation Neutron Source (SNS)** 

NANOSCALE SCIENCE RESEARCH CENTERS

Brookhaven National Laboratory

Sandia National Laboratories and

Los Alamos National Laboratory

Oak Ridge National Laboratory

Argonne National Laboratory

The Molecular Foundry (TMF)

Center for Nanoscale Materials (CNM)

Lawrence Berkeley National Laboratory

Center for Functional Nanomaterials (CFN)

Center for Integrated Nanotechnologies (CINT)

Center for Nanophase Materials Sciences (CNMS)

Oak Ridge National Laboratory

Oak Ridge National Laboratory

Linac Coherent Light Source (LCLS)

SLAC National Accelerator Laboratory

National Synchrotron Light Source II (NSLS-II)

Stanford Synchrotron Radiation Lightsource

SLAC National Accelerator Laboratory

Argonne National Laboratory

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**NEUTRON SOURCES** 

National Spherical Torus Experiment Upgrade (NSTX-U) Princeton Plasma Physics Laboratory

#### High Energy Physics (HEP)

- Facility for Advanced Accelerator Experimental Tests (FACET) SLAC National Accelerator Laboratory
- Fermilab Accelerator Complex Fermi National Accelerator Laboratory

#### Nuclear Physics (NP)

- Argonne Tandem Linac Accelerator System (ATLAS)
  - Argonne National Laboratory
- Continuous Electron Beam Accelerator Facility (CEBAF) Thomas Jefferson National Accelerator Facility
- Facility for Rare Isotope Beams (FRIB)
- Michigan State University
- Relativistic Heavy Ion Collider (RHIC) Brookhaven National Laboratory

#### Accelerator R&D and Production (ARDAP)

Accelerator Test Facility (ATF)
 Brookhaven National Laboratory

#### science.osti.gov/BES

# The ASCR Facilities are Scientific User Facilities





# The ASCR Facilities are Scientific User Facilities



#### Energy.gov/science

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Science

# The Office of Science Research Portfolio

Advanced Scientific Computing Research	<ul> <li>Delivering world leading computational and networking capabilities to extend the frontiers of science and technology</li> </ul>
Basic Energy Sciences	<ul> <li>Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels</li> </ul>
Biological and Environmental Research	<ul> <li>Understanding complex biological, earth, and environmental systems</li> </ul>
Fusion Energy Sciences	<ul> <li>Supporting the development of a fusion energy source and supporting research in plasma science</li> </ul>
High Energy Physics	<ul> <li>Understanding how the universe works at its most fundamental level</li> </ul>
Nuclear Physics	<ul> <li>Discovering, exploring, and understanding all forms of nuclear matter</li> </ul>
Isotope R&D and Production	<ul> <li>Supporting isotope research, development, production, processing and distribution to meet the needs of the Nation</li> </ul>
Accelerator R&D and Production	<ul> <li>Supporting new technologies for use in SC's scientific facilities and in commercial products</li> </ul>



### ASCR Facilities provide world-leading computing, data, and networking infrastructure for extreme-scale science while advancing U.S. competitiveness

#### High Performance Computing Facilities: ALCF, OLCF, NERSC





Leadership Computing Facilities (ALCF, OLCF): Unique national HPC resources for extreme-scale applications, delivering the exascale (10<sup>18</sup>) era of supercomputing



High Performance Production Computing Facility (NERSC): Dedicated HPC resource for the Office of Science research community, serving many thousands of users annually

#### **High Performance Network Facility: ESnet**



#### **Energy Sciences Network (ESnet):**

Connects all DOE national labs and dozens of other DOE sites to 150+ global research networks, commercial cloud providers, and the internet

Engineered for lossless transmission of huge data flows



# **ASCR – over 70 years of Advancing Computational Science**

**Beginnings:** During the Manhattan Project, John Von Neumann advocated for the creation of a Mathematics program to support the continued development of applications of digital computing



Over 40+ years, ASCR has a rich history of investment in computational science and applied mathematics research, and revolutionary computational and network infrastructure.



#### WHY COMPUTATIONAL SCIENCE?

- Computational science adds a third pillar to researcher's toolkit along side theory and experiments
- Computational science is essential when experiments are too expensive, dangerous, time-consuming or impossible
- Computational science facilitates idea-to-discovery that leads from equations to algorithms
- Virtually every discipline in science and engineering has benefited from DOE's sustained investments in computational science

The ASCR Facilities ecosystem began with the National Magnetic Fusion Energy Computing Center (later renamed NERSC) (1974) and ESnet (1985).





## **ASCR Facilities:** History



Ewing "Rusty" Lusk at ANL's Advanced Computing Research Facility which fielded an array of early parallel systems.





to address the grand challenge applications listed ORNL's Intel Paragon system was installed in 1995, comprising 3,072 processors to support research into Grand Challenge problems.

#### ASCR@40: Highlights and Impacts of ASCR's Programs

### Today: Exascale systems NERSC > 10,000 users! ESnet6 deployed

#### Aurora at Argonne







### **ASCR HPC system lifecycle timeline 2022-2035**

When "accepted," a system enters a five-year operations window (green bar); the red bar indicates a possible 6<sup>th</sup> year life extension.





# ASCR Resources at the LCFs: See the INCITE website doeleadershipcomputing.org





### The breadth of exascale-ready applications is remarkable; indicative of a sea change in computing abilities for DOE and the nation





### The ASCR Facilities user community is broad BOEING 🛆 Altair 🛛 🖊 Altair Chevron ECHNOLOGIES **E**%onMobil Ebbi GOOD KatRisk Lilly P&G Raytheon Technologies tae Technologies Whirlpool Nestinghouse NOAR NIH National Institutes of Health



# **High Performance Computing Allocation Programs**

			ERCAP	Director's Discretionary
Allocation Program Mission	Advance science and engineering	Advance DOE mission priorities; respond to national emergencies	Advance DOE Office of Science and SBIR/STTR research	Advance science and engineering
Allocatable Time	ALCF, OLCF: 60% NERSC: N/A	ALCF, OLCF: 30% NERSC: 10%	ALCF, OLCF: N/A NERSC: 80%	ALCF, OLCF: 10% NERSC: 10%
Managing Office	ALCF/OLCF	ASCR	DOE Office of Science Programs, SBIR/STTR	Each Facility
Award Duration	One year	One year (offset 6 months relative to INCITE)	One year	One year

For more information, see: <a href="https://science.osti.gov/ascr/Facilities/Accessing-ASCR-Facilities">https://science.osti.gov/ascr/Facilities/Accessing-ASCR-Facilities</a>



The best and most current information about ASCR Facility resources available to you are at the Facilities' websites:

### **Resource descriptions:**

- ALCF: <u>https://www.alcf.anl.gov/alcf-resources</u>
- OLCF: <u>https://www.olcf.ornl.gov/olcf-resources/</u>
- NERSC: <u>https://www.nersc.gov/systems/computational-systems-table/</u>

### Training opportunities and events:

- OLCF: <u>https://www.olcf.ornl.gov/for-users/training/</u>
- ALCF: <u>https://www.alcf.anl.gov/events</u>
- NERSC: <u>https://www.nersc.gov/events/calendar/</u>



# Additional information about allocation programs, from the Leadership Computing Facility perspective

Katherine Riley, Director of Science at ALCF and INCITE Program Manager



LCF Allocation Programs	INCITE	60%	A	LCC <u>30</u>	Director's 10% Discretionary	
Mission	Mission High-risk, high-payoff science that requires LCF-scale resources*		High-risk, high-payoff science aligned with DOE mission		Proposal preparation Strategic LCF programs ECP	
Call	1x/year – Opens Closes Jur	in April, ie	1x/year – Ope Closes	ens in November, s February	Rolling	
Duration	Duration 1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical # Projects	Typical # Projects10-30 projects/resource (system dependent)		5-15 projects/resource		~100 of projects/resource	
Average Award Range	~700K Frontier nod ~700K Aurora node ~200k Polaris nod	le-hours e-hours* e-hours	~700K Fron ~700K Auro ~100K Pola	tier node-hours ora node-hours* oris node-hours	~10K Frontier node-hours ~10K Aurora node-hours* ~1-2K Polaris node-hours	
<b>Review Process</b>	Scientific Comp Peer-Review Readi	utational ness	Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed By	INCITE management (ALCF & OL	t committee CF)	DOE Offic	ce of Science	LCF management	
Readiness	High		Medium to High		Low to High	
Availability		Open to all s	cientific resear	chers and organiz % of resource	ations	

# **ALCF Allocation Programs**



#### **INCITE:** Innovative and Novel Computational Impact on Theory and Experiment

- Yearly call with computational readiness and peer reviews
- Open to all domains and user communities

#### ALCC: ASCR Leadership Computing Challenge

- Yearly call with peer reviews
- Focused on DOE priority
- Exascale Computing Project (ECP)

#### **DD: Director's Discretionary Program**

- Rapid, small allocations for project prep and immediate needs
- Readiness Programs
- Strategic Program
- Proprietary Projects



### DD Director's Discretionary

- **Purpose:** A "first step" for projects working toward a major allocation
- Eligibility: Available to all researchers in academia, industry, and other research institutions
- **Review Process:** Projects must demonstrate a need for highperformance computing resources; reviewed by ALCF
- Award Size: Low 10 thousand of node-hours
- Award Duration: 3-6 months, renewable
- Total percent of ALCF resources allocated: 10%

• Award Cycle Ongoing (available year-round)



# Applying to DD

• Process is designed to be quick

—Short application, ~2 week turn around

- Demonstrate a need for LCF resource
- Evaluate viability and porting to LCF resources
- Work toward an INCITE or ALCC



The ALCF Director's Discretionary (DD) program is dedicated to helping researchers prepare for a major allocation award through DOE's INCITE and ALCC programs. DD projects allow users to improve application performance to maximize scientific application efficiency and productivity on the ALCF's leadership computing platforms. Projects must demonstrate a need for leadership-class resources.

Open to researchers from industry, academia, and government agencies, DD awards are available year-round and are usually between three and six months in duration. The size of the award varies based on the application and its readiness/ability to scale.

#### Apply for a DD award

#### Application Details

Eligibility:	Available to researchers from universities, industry, and government agencies DOE sponsorship is not required.		
Award size:	Small		
Duration:	3-6 months (renewable)		
Allocation cycle:	Ongoing (available year-round		
Quarterly reports:	No		
End of allocation reports:	No		

# ALCC ASCR Leadership Computing Challenge

- The DOE's ALCC program allocates resources to projects directly related to the DOE's energy mission, as well as national emergencies, and for broadening the community of researchers capable of using leadership computing resources.
- Eligibility: Available to researchers in academia, industry, and other research institutions
- Review process: DOE peer reviews all proposals for scientific/technical merit; appropriateness of approach; and adequacy of personnel and proposed resources
- Award size:

  - ~ 250K 1M Aurora node-hours
- Award duration: 1 year
- Total percent of ALCF resources allocated: 20-30%

• Award Cycle July 1 to June 30

Nov Call Plan for LOI

