



U.S. DEPARTMENT OF  
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# ASCR Leadership Computing Challenge 2022-23 Awards

ASCAC Meeting

Jordan Thomas

July 21, 2022

# ASCR High Performance Computing (HPC) and Networking Facilities

World leading capabilities spanning supercomputing, data analysis, data transport & testbeds



Argonne Leadership Computing Facility



Oak Ridge Leadership Computing Facility

## Leadership Computing: Extreme-scale resources for the nation

- ALCF and OLCF provide two HPC architectures for technological diversity
- ~3,000 users per year; multiple #1 Top500 rankings over program history
- Emphasis on science and technology applications that use full system capability
- Resources allocated predominantly by competitive merit review
- Current upgrade projects: OLCF-5 **Frontier** (2021-2022) and ALCF-3 **Aurora** (2022-2023)



NERSC at LBNL

## High Performance Production Computing: A dedicated SC resource

- NERSC's legacy of enabling DOE research with HPC stretches back to 1974
- ~8,000 users per year; NERSC also provides a 200 PB data storage archive
- Emphasis on support for the broadest set of science applications
- Resources allocated predominantly by SC Science Programs to their grantees
- Current upgrade project: NERSC-9 **Perlmutter** (2021-2022)

## Advancing U.S. Competitiveness

Every ASCR HPC system procurement includes R&D to drive innovation across the U.S. vendor community.

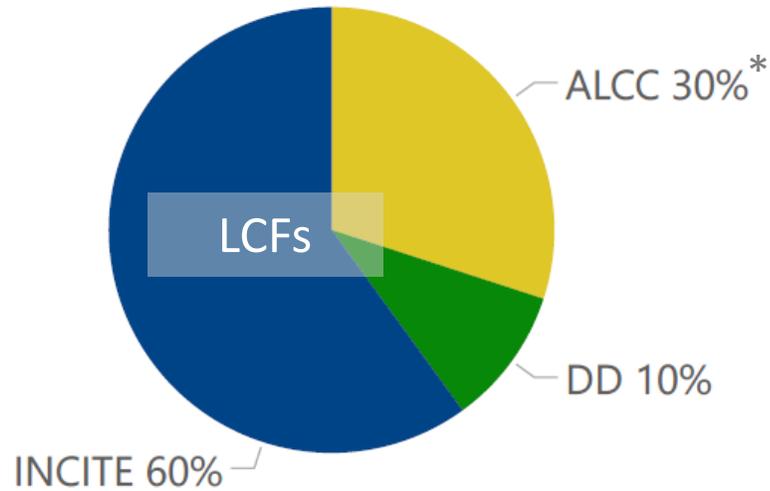
LCFs constitute a global competitive HPC advantage.



## High Performance Networking: A superhighway for extreme-scale data

- Connects all DOE national laboratories and other DOE sites to global research networks, cloud providers, and the internet
- Many tens of thousands of individual users; ESnet provides DOE the ability to move massive data losslessly
- An open network with high capacity (400+ Gbps), low latency, and innovative services tuned for extreme-scale data
- Transmitted more than one Exabyte (one billion Gigabytes) in the last 12 months; ESnet Testbed enables open R&D
- Current upgrade project: **ESnet6** (2022-2023), a Terabit-scale network with software programmable service orchestration

# ASCR HPC Resource 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
- Large allocations

## ERCAP: Energy Research Computing Allocations Process

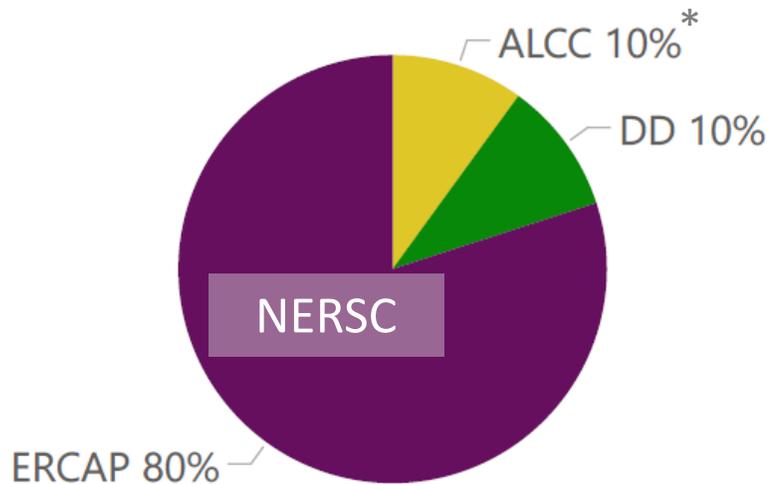
- Yearly call with peer review
- Open only to SC Program Offices
- Small-to-medium allocations

## ALCC: ASCR Leadership Computing Challenge

- Yearly call with peer reviews
- Focused on DOE priorities
- Small-to-medium allocations

## DD: Director's Discretionary Program

- Rapid allocations for project preparation and immediate needs
- Small allocations



\*Includes ECP-readiness allocations and projects

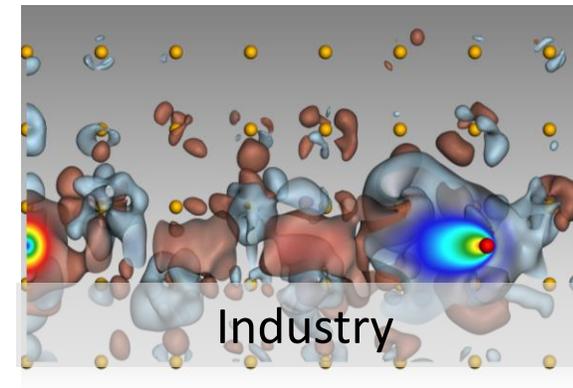
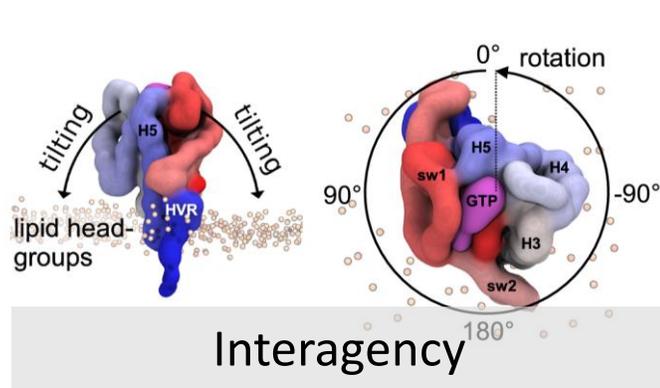
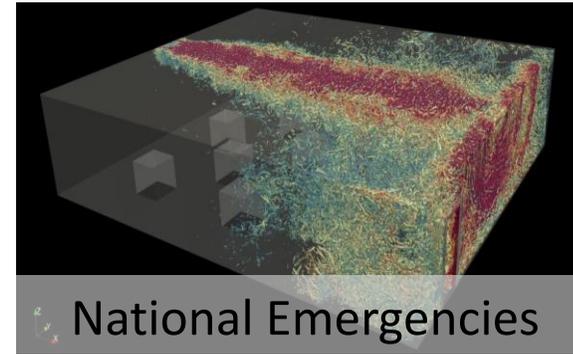


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# The ALCC Program Strives to Balance a Broad Range of Priorities

The ASCR Leadership Computing Challenge (ALCC) is an allocation program for projects of interest to the Department of Energy (DOE), with an emphasis on high-risk, high-payoff scientific campaigns enabled via high-performance computing (HPC) in areas directly related to the **DOE mission**, that respond to **national emergencies**, or that **broaden the community of researchers** capable of using leadership computing resources.



(Left) An impressionistic rendition of helimagnetism. LBNL

(Middle-Top) Energy-Efficient Windows. LBNL

(Middle-Bottom) RAS -- a signaling protein associated with the cell membrane that is mutated in up to 30% of human cancers. LLNL..

(Right-Top) Covid-19 spread simulation in a classroom. ANL, ORNL.

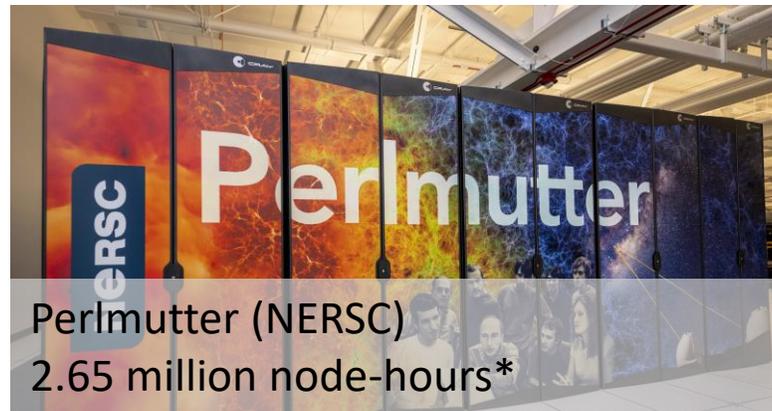
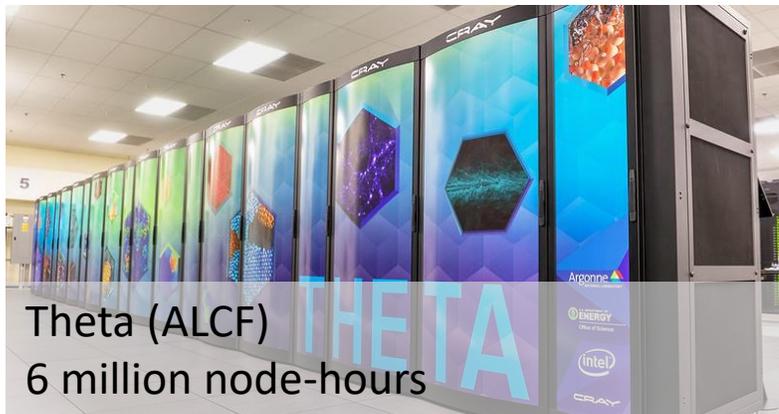
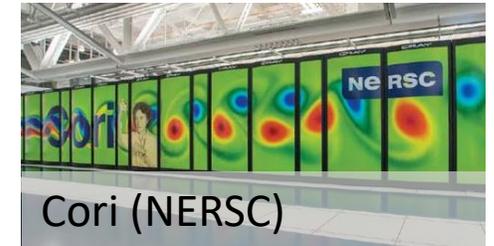
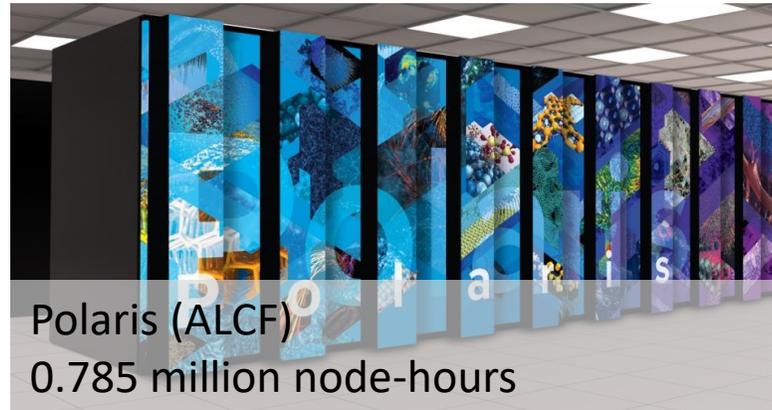
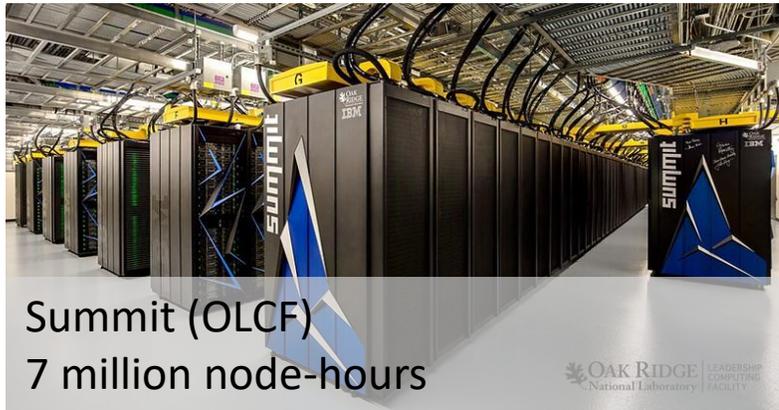
(Right-Bottom) Electronic Response to Particle Radiation in Condensed Matter. ANL.



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# ALCC 2022 Resources



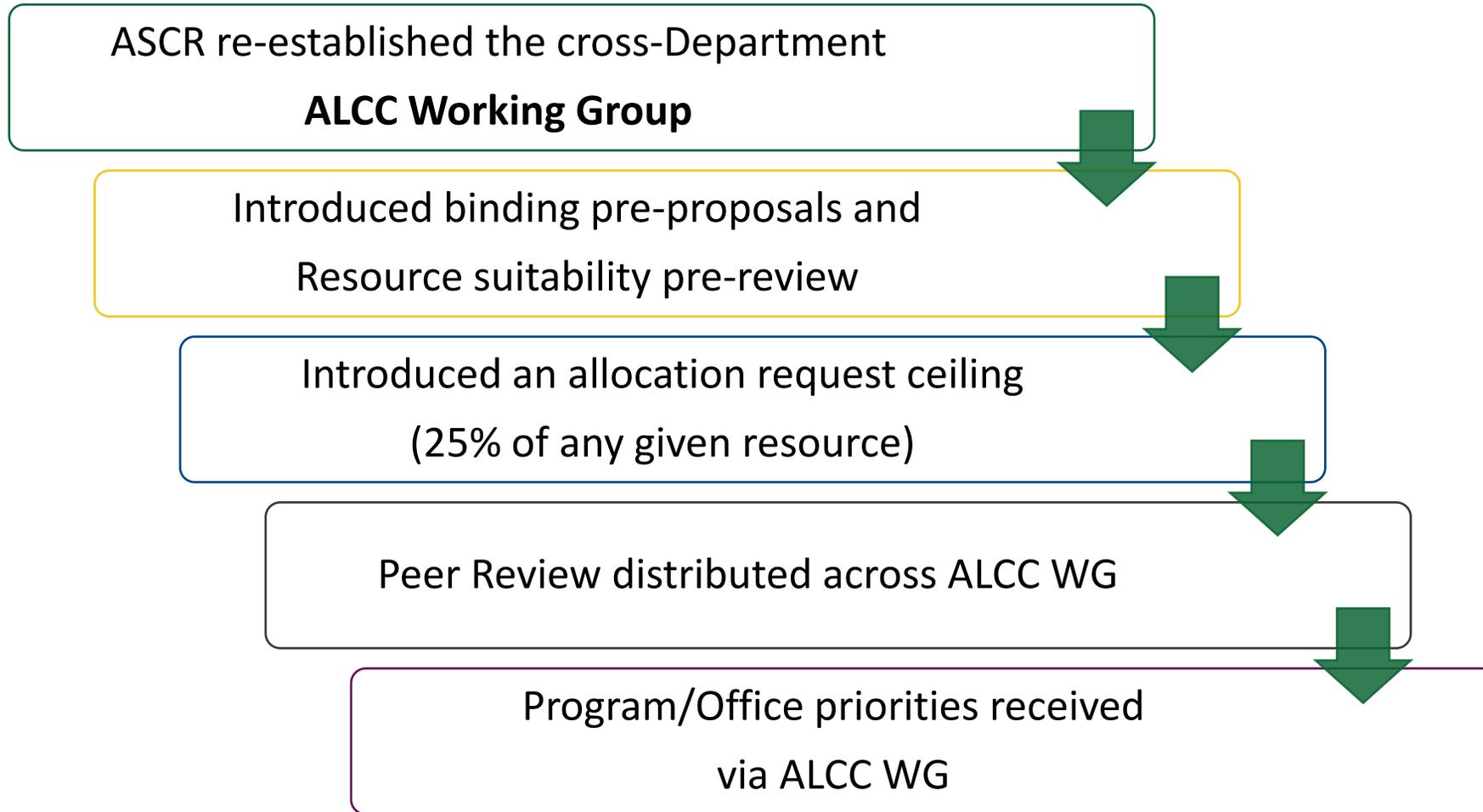
\*Split between CPU and GPU systems



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# The ALCC Program Process was revised in 2021 (same process for 2022)



# 2022 ALCC Process Timeline



# Submission Metrics

## Pre-Proposals

- 100 Submitted Pre-Proposals (87 last year)
- 2 Discouraged, 98 Encouraged

## Proposals

- 87 Submitted Proposals (76 last year)
- 57% Laboratory (47%), 36% University (40%), 5% Industry (8%), 2% Other (5%)

## Selected Projects

- 45 Selected Projects (41 last year)
- 52% Laboratory (45%), 42% University (41%), 4% Industry (7%), 2% Other (7%)



# 2022-23 ALCC Award Portfolio: An Overview

Number of Projects

45

Million Hours Awarded

18.0

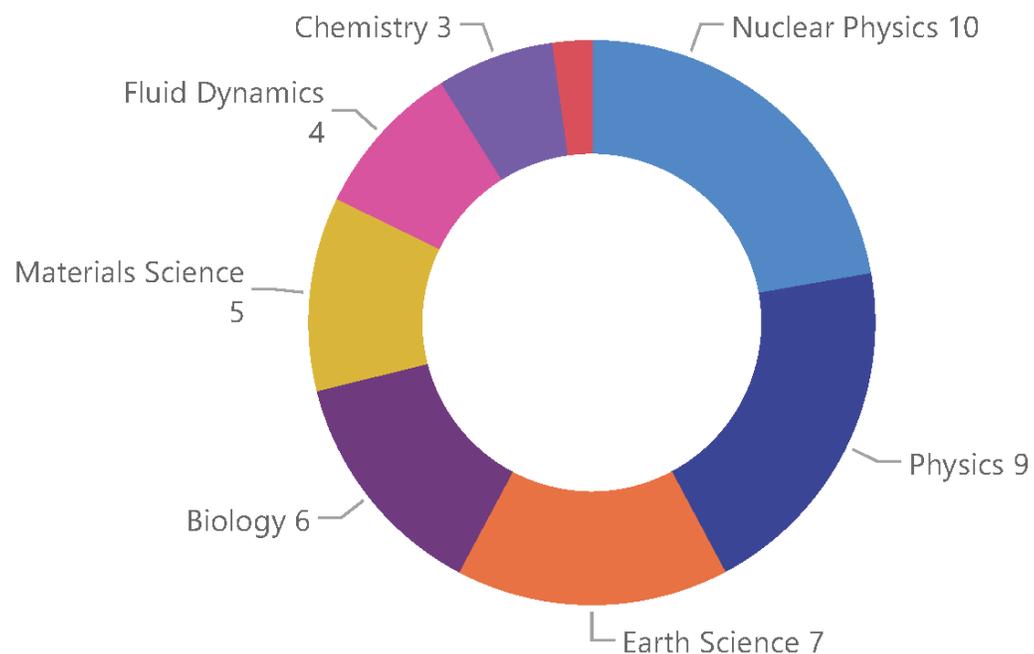
Previous ALCC Awardees

19

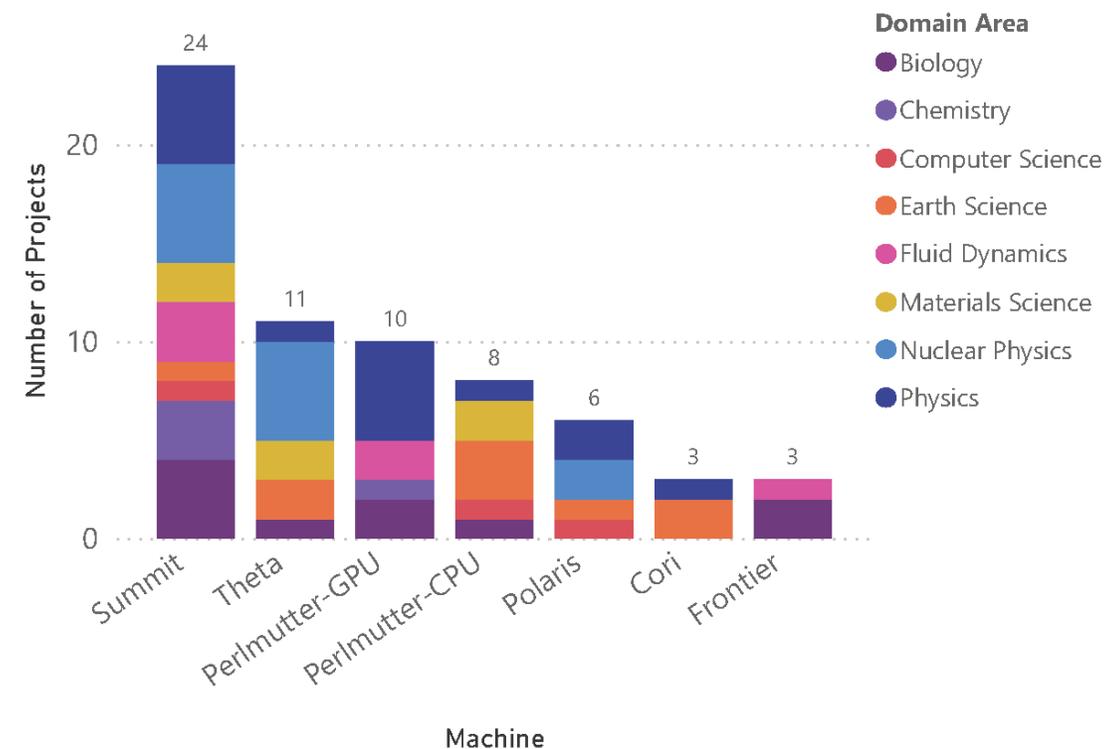
Unique Universities

16

Number of Projects by Domain Area



Number of Projects per HPC Resource

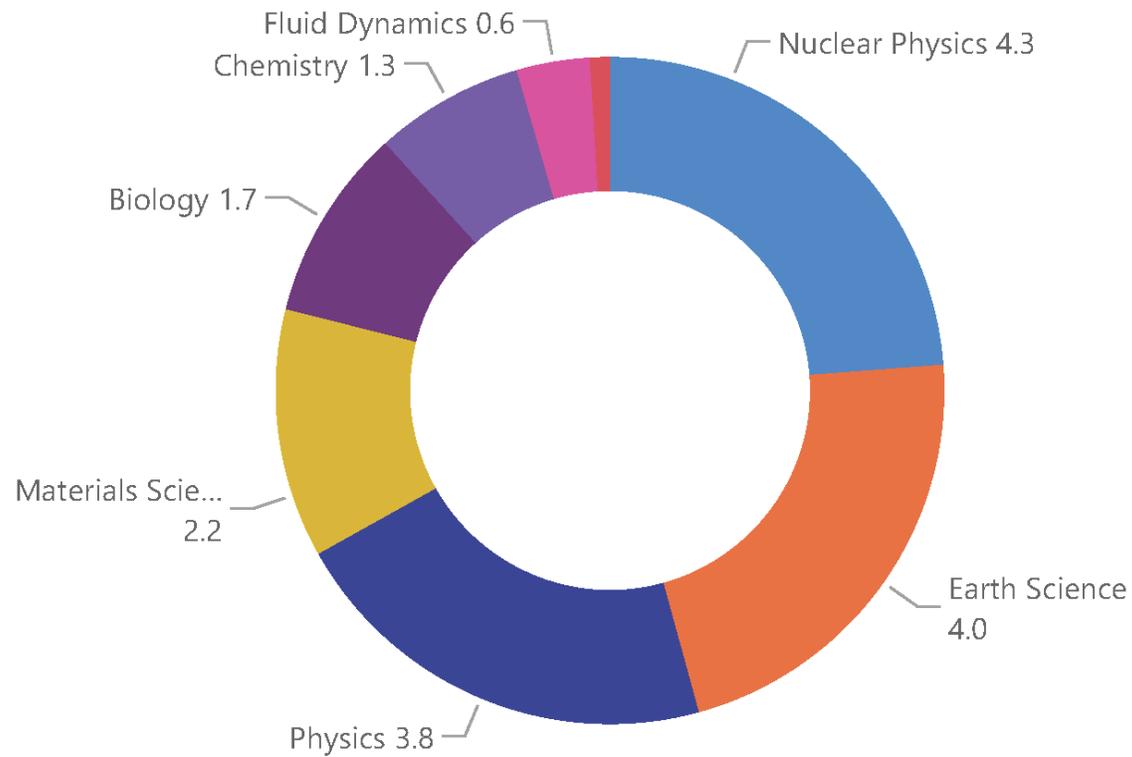


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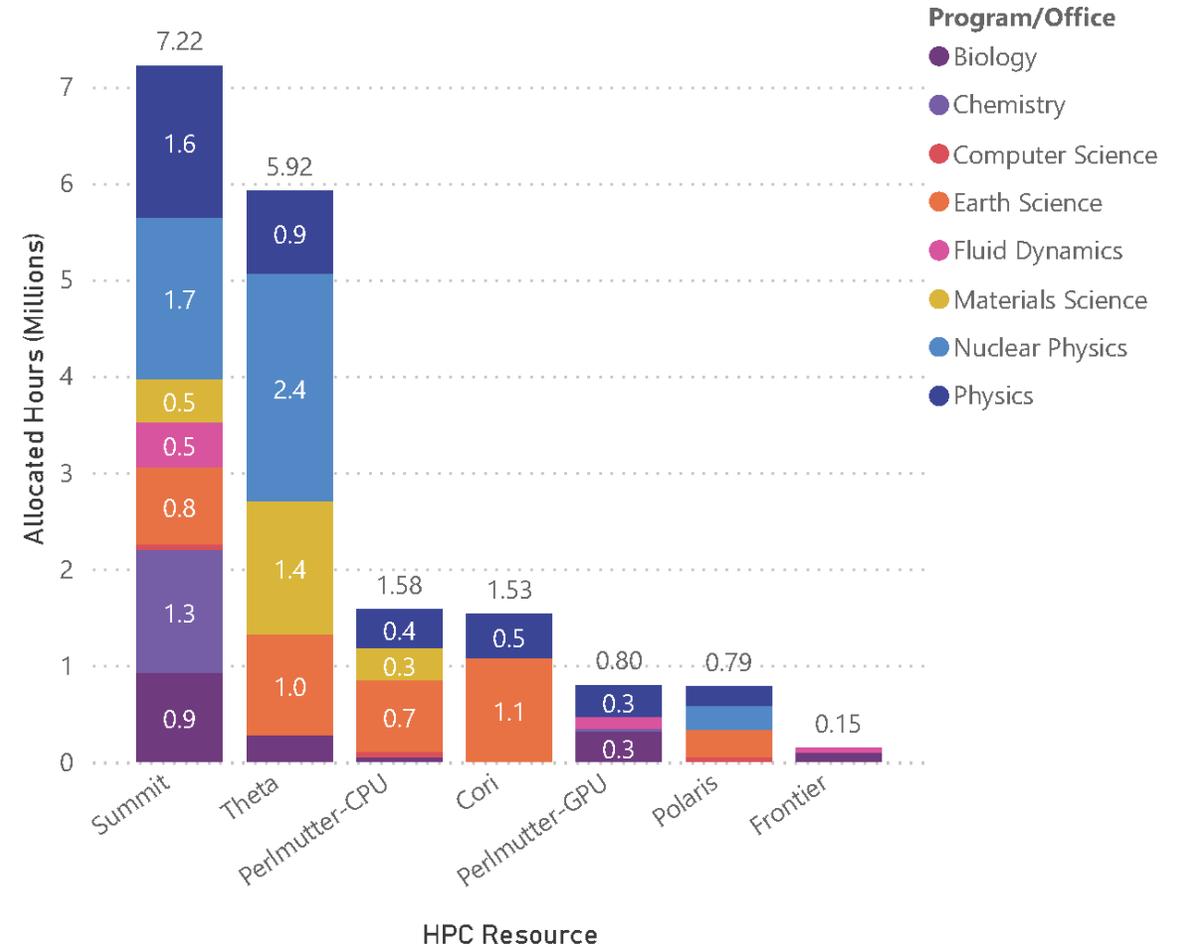
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# 2022-23 ALCC Award Portfolio: An Overview

Allocated Hours (Millions) Per Program/Office



Allocated Hours per HPC Resource



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# Featured Projects

## **Improved Seismic Hazard Modeling Using Physics-based Simulations**

Christine Goulet

University of Southern California

Seismic risk reduction is a long-term endeavor that requires research programs focused on reducing uncertainties at various steps of the evaluation process, starting from the hazard. The reduction of uncertainties will lead to more effective engineering designs and reduce financial losses and human casualties due to earthquakes. Thus, one of the goals of the Southern California Earthquake Center (SCEC) is to develop accurate assessments of ground motions and fault displacement for future earthquakes.

Allocation: 475,000 node-hours on Summit  
783,000 node-hours on Cori

## **Particle-in-cell simulations of beam-driven, field-reversed configuration Plasmas**

Richard Magee

TAE Technologies, Inc.

This project will advance the understanding of the FRC plasma, an important alternative confinement concept in magnetic fusion energy with tangential tie-ins to astrophysical phenomena and emerging propulsion technologies, as well as expand the HPC usage base in the private fusion sector, fostering future private-public ventures in the fusion industry.

Allocation: 400,000 node-hours on Theta



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# Featured Projects

## Mitigating Climate Change Through Zero Carbon Fuels

Jacqueline Chen  
Sandia National Laboratories

Mitigating climate change while providing our nation's transportation and power generation needs are key to energy and environmental security. New e-fuels and hydrogen rich fuels provide a near zero-carbon alternative to fossil fuels for gas turbine engines for power generation and for compression ignition engines for marine shipping. Fundamental understanding of gas-phase chemistry-transport interactions with zero-carbon fuels, and especially NO<sub>x</sub> formation with ammonia/hydrogen blends, is relevant to the DOE BES Gas Phase Chemical Physics mission.

Allocation: 400,000 node-hours on Summit

## Privacy-preserving Transformer models for clinical natural language Processing

Heidi Hanson  
Oak Ridge National Laboratory

A notable challenge in analysis of clinical text is that it contains protected health information (PHI) and AI models must be trained securely using. However, as the trained models may memorize PHI from our data, they cannot be publicly released to the biomedical research community. Sharing these models is nonetheless important, both to the broader impact of this project and to the explicit aims of the DOE-NCI partnership. Accordingly, in this project, we aim to address the additional challenges related to training Transformer models on clinical text data that contains PHI.

Allocation: 150,000 node-hours on Summit  
30,000 node-hours on Frontier



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# 2022-2023 ALCC Portfolio: Physics

Proposal Title	PI	PI Institution	Resource(s)	Allocation
Exploring pedestal structure via the electromagnetic gyrokinetic framework	Jeff Candy	General Atomics	Summit Perlmutter-GPU	0.07 0.06
Energy partition and particle acceleration in laboratory magnetized shocks	Frederico Fiuza	SLAC National Accelerator Laboratory	Theta	0.86
High Precision Hadronic Vacuum Polarization Contribution to the Muon Anomalous Magnetic Moment using Highly Improved Staggered Quarks	Steven Gottlieb	Indiana University	Summit Polaris Perlmutter-GPU	1 0.1 0.1
Gyrokinetic Prediction of Burning Plasma Profiles Enabled by Surrogate Modeling	Nathan Howard	Massachusetts Institute of Technology	Perlmutter-GPU	0.075
Using GPU to reconstruct LHC collisions recorded with the CMS detector	Dirk Hufnagel	Fermilab	Summit	0.05
Cosmological Hydro Simulations to Explore the High and Low-Redshift Universe	Zarija Lukic	Lawrence Berkeley National Laboratory	Summit Polaris Perlmutter-GPU	0.05 0.1 0.05
Optimization studies of LBNF neutrino beamline and hadron absorber complex	Igor Rakhno	Fermi National Accelerator Laboratory	Cori	0.45
Simulating Collapsar Accretion Disks, Outflows, and Nucleosynthesis	Alexander Tchekhovskoy	Northwestern University	Summit Perlmutter-GPU	0.4 0.04
Laser-plasma instability mitigation using broadband lasers	Han Wen <sup>α</sup>	Laboratory for Laser Energetics, University of Rochester	Perlmutter-CPU	0.4



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# 2022-2023 ALCC Portfolio: Nuclear Physics

Proposal Title	PI	PI Institution	Resource(s)	Allocation
The spectrum and structure of hadrons	Robert Edwards	Jefferson Lab	Polaris	0.3
Monte Carlo neutron transport for high burnup/high enrichment nuclear fuel	Steven Hamilton	Oak Ridge National Laboratory	Summit	0.25
Informing Forensics Investigations of Nuclear Materials	Sara Isbill	Oak Ridge National Laboratory	Summit	0.175
Particle-in-cell simulations of beam-driven, field-reversed configuration plasmas	Jaeyoung Magee	TAE Technologies, Inc.	Theta	0.4
High-Fidelity Flow Data for Multiscale Bridging: Year 2	Elia Merzari	Pennsylvania State University	Summit	0.25
Predictive Simulations of Inertial Confinement Fusion Ablator Materials	Ivan Oleynik	University of South Florida	Polaris	0.15
HFIR DNS simulations	Emilian Popov	ORNL	Theta	0.224
Short Range Correlations from a Quantum Monte Carlo perspective	Noemi Rocco	Fermi National Accelerator Laboratory	Theta	0.73
High-Fidelity CFD Simulations for Next Generation Nuclear Reactor Designs	Dillon Shaver	Argonne National Lab	Summit Theta Polaris	0.4 0.4 0.1
Investigation of Flow and Heat Transfer Behavior in Involute Plate Research Reactor with Large Eddy Simulation to Support the Conversion of Research Reactors to Low Enriched Uranium Fuel	Yiqi Yu	Argonne National laboratory	Theta	0.6



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# 2022-2023 ALCC Portfolio: Earth Science & Fluid Dynamics

Proposal Title	PI	PI Institution	Resource(s)	Allocation
Advancing Watershed System Science using ML and Process-based Simulation	Ethan Coon	Oak Ridge National Laboratory	Perlmutter-CPU	0.18
Improved Seismic Hazard Modeling Using Physics-based Simulations	Christine Goulet	University of Southern California	Polaris Cori	0.285 0.783
Shock Turbulent Boundary Layer Interaction in Supercritical CO2 Flows	Sanjiva Lele	Stanford University	Summit	0.18
Terrestrial ecosystem carbon cycle of the conterminous U.S.	Jinxun Liu	U.S. Geological Survey, Western Geographic Science Center	Cori	0.3
E3SMv2 Smoothed Biomass Burning Large Ensemble	Gerald Meehl	NCAR	Perlmutter-CPU	0.26
Large-eddy simulations of dynamic stall in a boundary layer ingesting turbofan	Parviz Moin	Stanford University	Summit	0.15
High-Fidelity Simulations of Turbulent Aeroacoustics Enabling Sustainable Aviation	Stephan Priebe	GE Research	Summit Perlmutter-GPU Frontier	0.13 0.035 0.13
Modeling operating conditions in the US east coast offshore wind energy lease areas	Sara Pryor	Cornell University	Theta	0.142
Unlocking wind farm dynamics to secure a sustainable energy future	Michael Sprague	National Renewable Energy Laboratory	Summit	0.8
Simulation of flow and transport in desalination systems	David Trebotich	Lawrence Berkeley National Laboratory	Perlmutter-GPU	0.09216
A Climate Model Ensemble for Understanding Future Changes to Extreme Weather	Paul Ullrich	University of California, Davis	Theta Perlmutter-CPU	0.9 0.3



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# 2022-2023 ALCC Portfolio: Biology, Chemistry & Computer Science

Proposal Title	PI	PI Institution	Resource(s)	Allocation
AI-Driven Multiscale Investigation of RAS-RAF Activation Lifecycle	Harsh Bhatia	Lawrence Livermore National Laboratory	Summit	0.35
			Frontier	0.35
Mitigating Climate Change Through Zero Carbon Fuels	Jacqueline Chen	Sandia National Laboratories	Summit	0.4
Dynamics and decoherence of excited states in 2D systems for quantum technology	Mauro Del Ben	LBNL	Summit	0.1
			Perlmutter-GPU	0.025
Deep learning-enabled ab initio simulation of heterogeneous aqueous systems	Zachary Goldsmith	Princeton University	Summit	0.86
Privacy-preserving Transformer models for clinical natural language processing	Heidi Hanson	Oak Ridge National Laboratory	Summit	0.15
			Frontier	0.15
A Multiscale Surrogate Model for Fracture Evolution using DeepONet	George Karniadakis	Brown University	Summit	0.06
			Polaris	0.05
			Perlmutter-CPU	0.06
Probabilistic Comparative Modeling of Colorectal Cancer Screening Strategies	Jonathan Ozik	Argonne National Laboratory	Theta	0.283
Integrating HPC molecular simulation with neutron scattering to study complex biological systems	Loukas Petridis	Oak Ridge National Laboratory	Perlmutter-GPU	0.3
Proteome-scale structural and function prediction with deep learning	Jeffrey Skolnick	Georgia Tech Research Corporation	Summit	0.13
			Perlmutter-CPU	0.05
			Perlmutter-GPU	0.02
Automatic Histologic Diagnosis of Whole Slide Imaging at Scale	Hong-Jun Yoon	Oak Ridge National Laboratory	Summit	0.3



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# 2022-2023 ALCC Portfolio: Materials Science

Proposal Title	PI	PI Institution	Resource(s)	Allocation
Accelerated Discovery of Low-Cost Hydrogen-Resistant Alloys for Extreme Environments	Michael Gao	National Energy Technology Laboratory	Perlmutter-CPU	0.25
First-principles prediction of solute segregation at defects in Mg alloys	Vikram Gavini	University of Michigan	Summit	0.1765
Computational design of novel semiconductors for power and energy applications	Feliciano Giustino	The University of Texas at Austin	Theta	0.883
Microscopic Insight into transport properties of Li-battery electrolytes	Wei Jiang	Argonne National Laboratory	Theta	0.5
QMC-HAMM: From the nanoscale to the mesoscale	Lucas Wagner	University of Illinois at Urbana-Champaign	Summit Perlmutter-CPU	0.277 0.083



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# Considerations for Next Cycle/Year

## ALCC Working Group

- Increase representation across the DOE
- Refine review panel grouping to include cross-cutting initiative groups (Artificial Intelligence, ect.)

## Demographic Data Collection

- **Request demographic data from applicants so we can track and improve our diversity.**
- Request demographic data from reviewers.
- Track new users and renewal applicants.

## Strategic Plan and Goals

- Out-of-cycle ALCC proposal process and procedures
- Better define ALCC within ASCR allocations space
- **More resources and outreach for applicants**

