

Argonne Leadership Computing Facility

Accelerating Discovery and Innovation

Katherine M Riley
Director of Science, Argonne Leadership Computing Facility

www.anl.gov

Supercomputing Resources

Our supercomputers are 10 to 100 times more powerful than systems typically used for scientific research.



Computing Resource for 2019



Theta Cray XC40
4,392 nodes
281,088 cores
892 TiB RAM
Peak flop rate: 11.69 PF



Theta

Features Intel processors and interconnect technology, a new memory architecture, and a Lustre-based parallel filesystem – all integrated by Cray's HPC software stack

Iota Intel/Cray XC40
44 nodes
2,816 cores
8.9 TiB RAM
Peak flop rate: 117 TF

Firestone IBM Power8
2 nodes + K80 GPU
20 cores
128 GB RAM
Hybrid CPU/GPU

Cooley Cray/NVIDIA
126 nodes
1512 Intel Haswell CPU cores
126 NVIDIA Tesla K80 GPUs
48 TB RAM / 3 TB GPU

Storage Capability

Disk

- Theta: ~18 PB of GPFS/Lustre file system capacity; 9PB is GPFS and 9.2PB is Lustre.

Tape

- The ALCF has three 10,000-slot libraries using LTO 6 tape technology. The LTO tape drives have built-in hardware compression for an effective capacity of 36-60 PB.

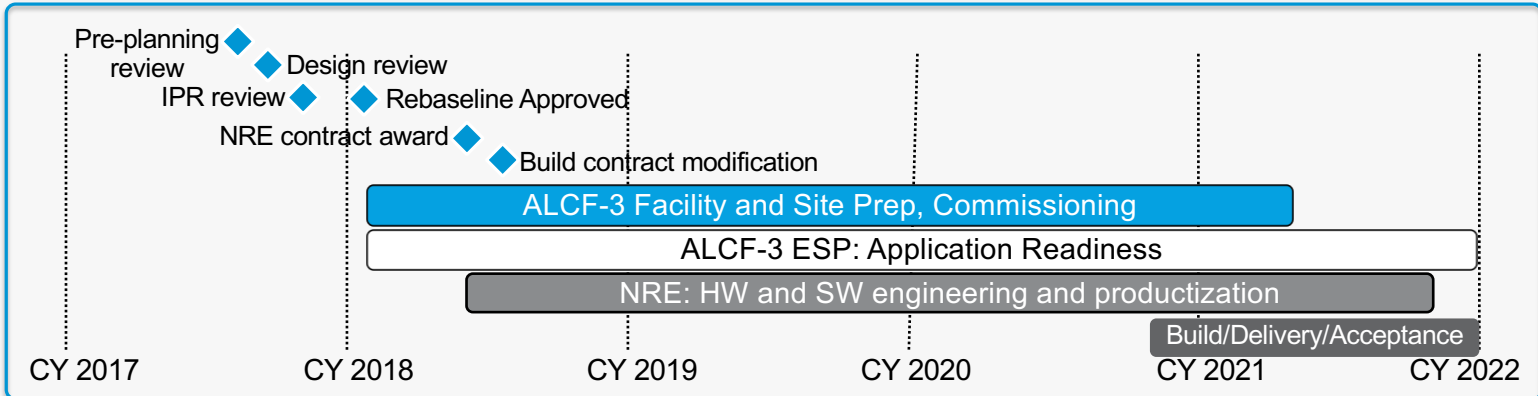
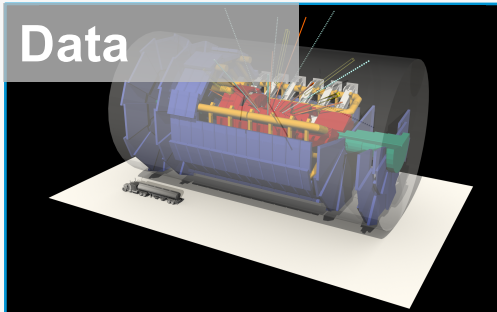
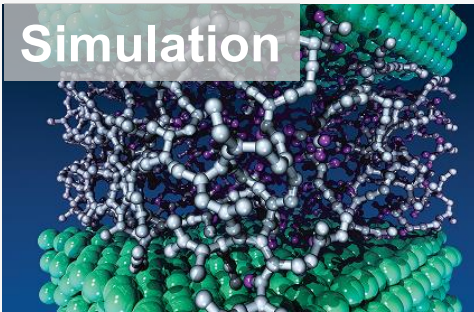
Aurora : Nations First Exascale Supercomputer

Intel supercomputer to be delivered in 2021

Over 1000 PF



Supporting the future of science





How Do Researchers Gain Access to ALCF?

We offer different pipelines based on your computational readiness. Apply to the allocation program that fits your needs.

- **Getting Started (DD)**
- **Major Awards (INCITE, ALCC)**
- **Targeted Projects (ADSP, ESP)**

Primary Allocation Programs for Access to the LCFs

Current distribution of allocable hours

20% Director's Discretionary
(Includes LCF strategic programs, ECP)



20% ASCR Leadership Computing Challenge

DOE/SC capability computing



60% INCITE

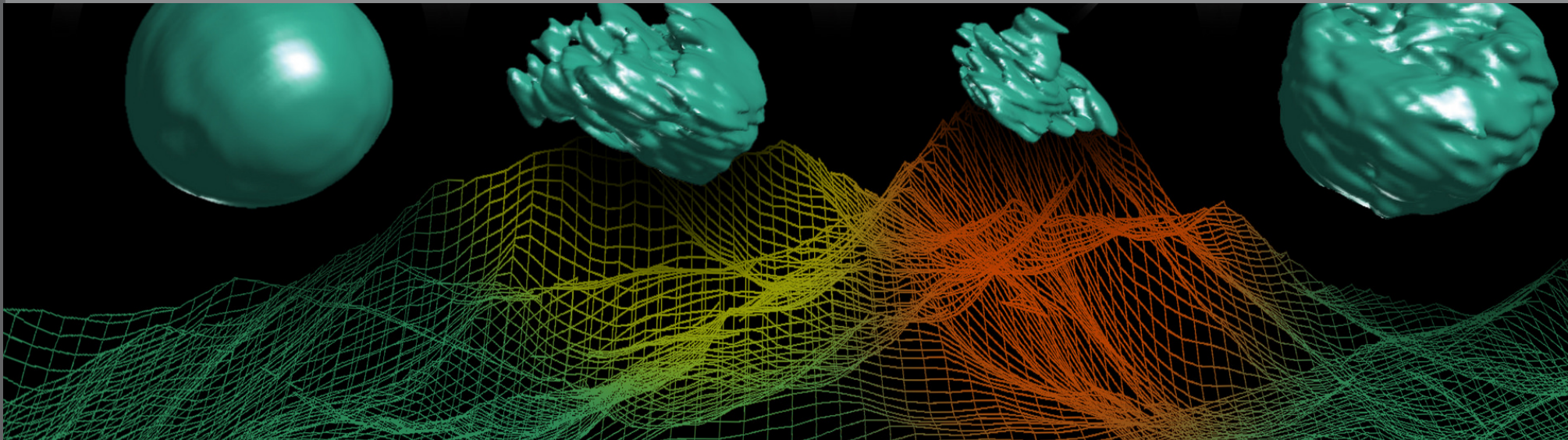
Leadership-class computing



Getting Started (DD)

Our Director's Discretionary (DD) allocation program provides researchers with small awards of computing time to "get started" on our computing resources while pursuing real scientific goals.

The DD allocation program allows users to prep their code so that it can take advantage of our massively parallel systems.



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 high-performance computing resources; reviewed by ALCF

Award Size: Low tens of thousands to the low millions of compute hours

Award Duration: 3-6 months, renewable

Total percent of ALCF resources allocated: 20%

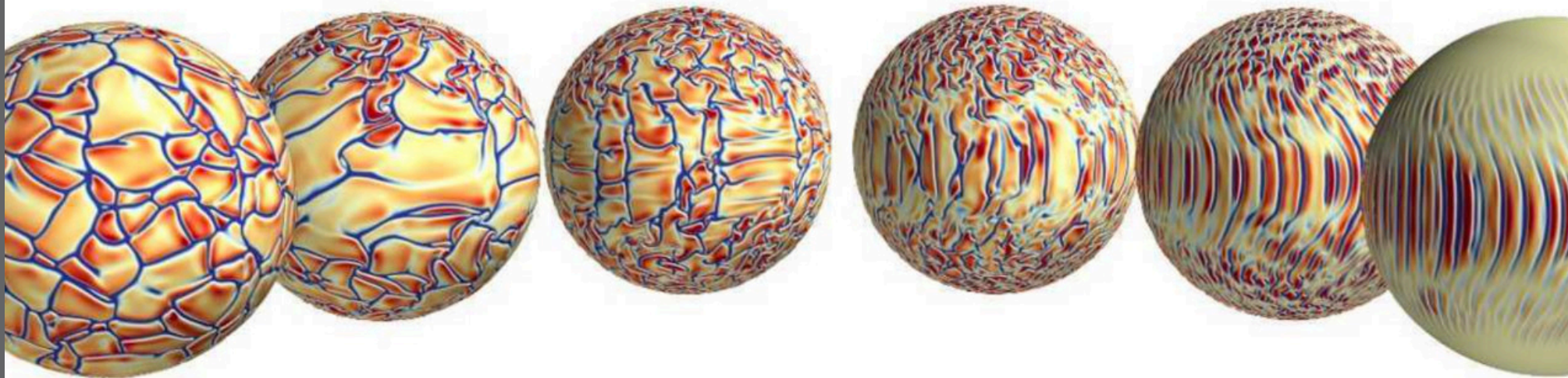
Award Cycle

Ongoing (available year round)

Major Awards (INCITE, ALCC)

Our major allocations provides users with computationally intensive, large-scale research projects time on our machines.

The programs conduct a two-part review of all proposals: a peer review by a panel of experts and a computational readiness review.



INCITE

Innovative & Novel Computational Impact on Theory and Experiment

The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering.

Eligibility: Available to researchers in academia, industry, and other research institutions

Review process: INCITE program conducts a two-part review of all proposals including a peer review by an international panel of experts, and a computational-readiness review

Award size: Low to high millions of core-hours

Award duration: 1-3 years, renewable

Total percent of ALCF resources allocated: 60%

Award Cycle

January 1 to December 31

What is INCITE?



Innovative and Novel Computational Impact on Theory and Experiment

INCITE promotes transformational advances in science and technology through large allocations of computer time, supporting resources, and data storage at the Argonne and Oak Ridge Leadership Computing Facilities (LCFs) for computationally intensive, large-scale research projects.



INCITE criteria

Access on a competitive, merit-reviewed basis*

1	Merit criterion
	Research campaign with the potential for significant domain and/or community impact
2	Computational leadership criterion
	Computationally demanding runs that cannot be done anywhere else: capability, architectural needs
3	Eligibility criterion
	<ul style="list-style-type: none">• Grant allocations regardless of funding source*• Non-US-based researchers are welcome to apply

*DOE High-End Computing Revitalization Act of 2004: Public Law 108-423

Twofold review process

	New proposal assessment	Renewal assessment
1	Peer review: INCITE panels <ul style="list-style-type: none"> • Scientific and/or technical merit • Appropriateness of proposal method, milestones given • Team qualifications • Reasonableness of requested resources 	<ul style="list-style-type: none"> • Change in scope • Met milestones • On track to meet future milestones • Scientific and/or technical merit
2	Computational readiness review: LCF centers <ul style="list-style-type: none"> • Technical readiness • Appropriateness for requested resources 	<ul style="list-style-type: none"> • Met technical/computational milestones • On track to meet future milestones
	Award Decisions <ul style="list-style-type: none"> • INCITE Awards Committee comprised of LCF directors, INCITE program manager, LCF directors of science, sr. management 	

Recent Trends in INCITE

Data, Learning and Nontraditional Uses of the Architecture

In addition to traditional computationally intensive simulation campaigns, INCITE encourages Data and/or Learning projects with unique data requirements (e.g. large scale data analytics) or workflow needs that can only be enabled by the LCFs.

- A “Learning” panel evaluated proposals that had significant machine / deep learning component to their campaign
- These proposals were also assessed by their scientific discipline peers as well

2019 award statistics, by system

	Titan	Summit	Mira	Theta
Number of projects*	20	30	21	16
Average Project	1.95 M	457 K	10.5 M	1.11 M
Median Project	1.41 M	357 K	8.00 M	1.00 M
Total Awards (node-hrs in CY2016)	39.0 M	13.7 M	220 B	17.8 M

* Total of 62 INCITE projects (many of the projects received time on a combination of Mira, Theta, Titan, and Summit)

** All reported in node-hours nature to each resource.

New proposals,* new PI's

*excluding renewal submittals

38% of the PI's had never before led an INCITE proposal

– 104 new proposals, 41 led by new PI's

- 20% of non-renewal projects awarded time led by new PI's
 - 41 new projects awarded, 8 led by new PI's

INCITE actively engages with new research teams through outreach such as workshops, email distributions, and individual networking.

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: Low to high millions of core-hours

Award duration: 1 year

Total percent of ALCF resources allocated: 20%

Award Cycle

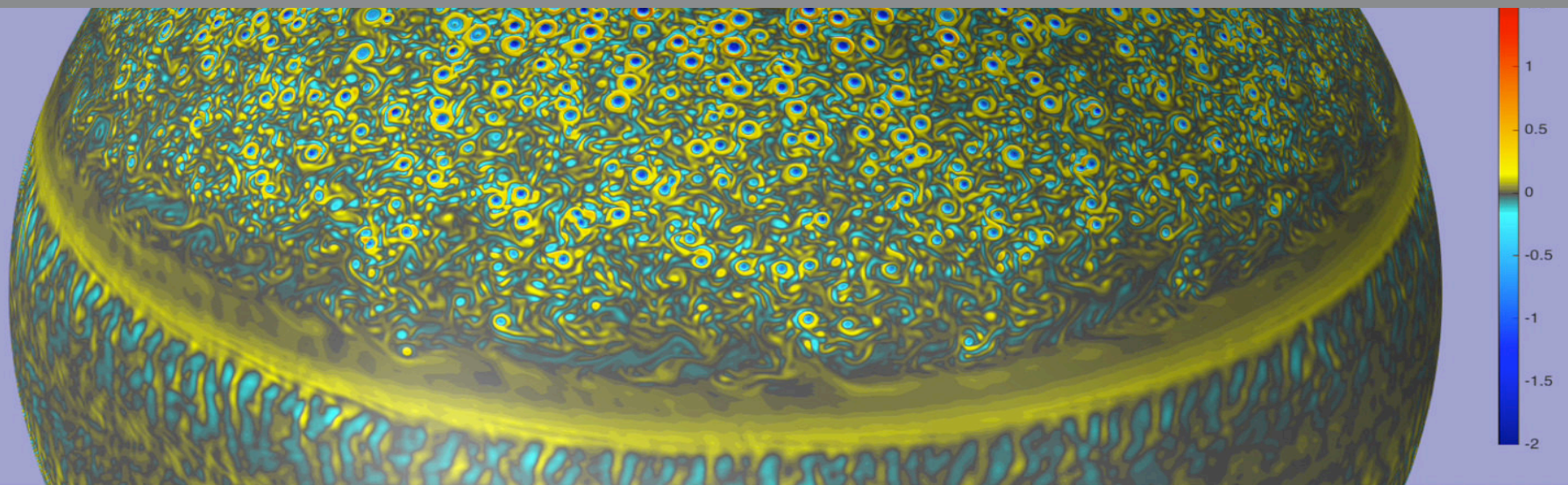
July 1 to June 30

LCF Allocation Programs	INCITE	60%	ALCC	20%	Director's Discretionary	20%
Mission	High-risk, high-payoff science that requires LCF-scale resources*		High-risk, high-payoff science aligned with DOE mission		Strategic LCF goals ECP	
Call	1x/year – (Closes June) <i>2019 Call Open</i>		1x/year – Closes February		Rolling	
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical Size	10-15 projects	1-3M node-hours	10-15 projects	0.5-2M node-hours	~100 of projects	<0.5M node-hours
Total Hours	~17.8M Theta		~6M node-hours Theta		~6M node-hours Theta	
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed By	INCITE management committee (ALCF & OLCF)		DOE Office of Science		LCF management	
Readiness	High		Medium to High		Low to High	
Availability	Open to all scientific researchers and organizations Capability > 20% of resource					

Targeted Projects (ADSP, ESP)

Our ADSP program is intended for projects hoping to gain insight into very large datasets produced by experimental, simulation, or observational methods.

Our ESP program is intended to help ready our next-generation supercomputers for production.



ADSP

ALCF Data Science Program

Targeted at big data science problems, ADSP aims to explore and improve a variety of computational methods that will help enable data-driven discoveries across all scientific disciplines.

Eligibility: Available to researchers in academia, industry, and other research institutions

Review process: Applications undergo a review process to evaluate potential impact, data scale readiness, diversity of science domains and algorithms, and other criteria

Award size: Low to high millions of core-hours

Award duration: 2 years

Award Cycle

October 1 to September 30

ESP

Early Science Program

As part of the process of bringing a new supercomputer into production, the ALCF hosts the Early Science Program (ESP) to ensure its next-generation systems are ready to hit the ground running.

The intent of the ESP is to use the critical pre-production time period to prepare key applications for the architecture and scale of a new supercomputer, and to solidify libraries and infrastructure to pave the way for other production applications to run on the system.

In addition to fostering application readiness, the ESP allows researchers to pursue innovative computational science projects not possible on today's leadership-class supercomputers.

Award Cycle

Determined by production timeline



Thank You!

Learn more at: alcf.anl.gov