Innovative and Novel Computational Impact on Theory and Experiment

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

The INCITE program provides awards of time on the Oak Ridge and Argonne Leadership Computing Facility (LCF) high performance computer systems for researchers to pursue transformational advances in science and technology. If you answer yes to the following questions, INCITE may be right for you. To begin the process, submit an RFI: http://hpc.science.doe.gov/allocations/incite

We invite prospective INCITE proposal authors to respond to our Request for Information (RFI) to inform the INCITE management of the proposal topics anticipated. To submit an RFI, search: DOE INCITE RFI

Is your science campaign outpacing the computing resources available to you?

Do you have a long-term vision for your research campaign, over a period of years rather than months?

Can you effectively use an INCITE-sized award, more than twenty million core-hours?

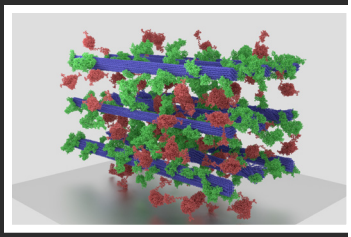
INCITE issues an annual call for proposals of high-impact, computationally intensive research campaigns in a broad array of science, engineering, and computer science domains. Individuals and teams of researchers from academia, national laboratories, and industry are eligible to apply. Awards of one-, two-, or three-years are granted.

INCITE awards are large – on the order of millions of core-hours – and selected by a peer review process. Campaigns chosen by the INCITE program typically cannot be performed anywhere else and require extremely large high performance computing systems, large awards of time, or the unique LCF architectural infrastructure in order to succeed.

INCITE supports research that answers key scientific or technical questions or points to new areas of research. Accomplishments by INCITE researchers are frequently seen in *Nature*, *Science*, and other highly visible journals. Contact us if you would like to learn more about LCF resources and the INCITE call for proposals.

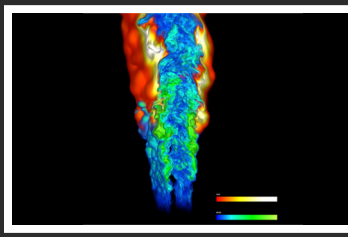
INCITE

SCIENCE HIGHLIGHTS



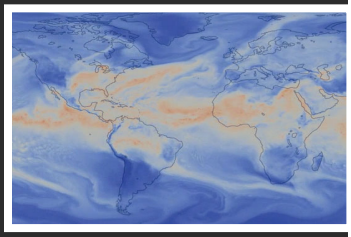
Biological Sciences

Jeremy Smith • Oak Ridge National Laboratory • 78 million core-hours
If cellulosic ethanol is to be an economical fuel alternative, researchers need a better understanding of its properties to combat its resistance to hydrolysis, the process by which it is broken down.



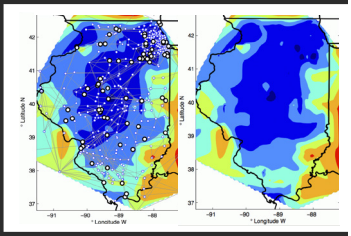
Chemical Sciences

Joseph Oefelein • Sandia National Laboratories • 100 million core-hours
State-of-the-art combustion simulations will allow the next generation of bio- and diesel fuels to burn more efficiently, reducing American dependence on foreign oil and curbing climbing carbon emissions.



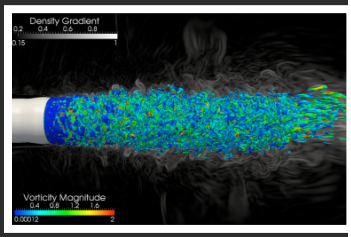
Earth Sciences

Warren Washington • University Corporation for Atmospheric Research • 215 million core-hours
By investigating the factors that led to the last great deglaciation, researchers hope to better discern carbon dioxide's role in today's climate.



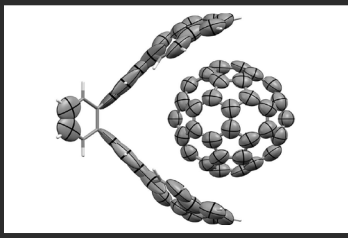
Energy Technologies

Mihai Anitescu • Argonne National Laboratory • 14 million core-hours
Novel optimization-under-uncertainty formulations of management of renewable energy sources may enable large percentages of wind penetration without significant increase in reserves or decrease in reliability.



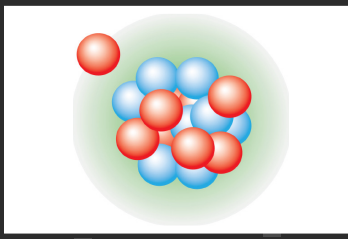
Engineering

Umesh Paliath • GE Global Research • 105 million core-hours
By predicting flow, more fuel-efficient and quieter wind turbines and jet engines can be developed and will improve engine life cycles.



Materials Science

Dario Alfe • University College London • 95 million core-hours
Using the Quantum Monte Carlo method, water can be modeled with unprecedented accuracy to yield insights applicable in aqueous chemistry across scientific disciplines.



Physics

James Vary • Iowa State University • 155 million core-hours
By calculating the number of isotopes that are theoretically possible under the laws of physics, researchers are one step closer to understanding the nuclear landscape and designing specific nuclei with unique properties.

Titan

Titan, a Cray XK7 supercomputer, is the primary computational resource within the Oak Ridge Leadership Computing Facility (OLCF). The Cray XK7 is a hybrid architecture where each individual compute node uses both a conventional 16-core AMD 6274 Opteron™ and an NVIDIA K20x (Kepler) GPU. Titan, with 18,688 of these hybrid compute nodes, has a theoretical peak computational performance of more than 27 PFLOPS. The XK7 design overcomes the power and space limitations inherent in previous generations of high performance computers. Each of these compute nodes is interconnected with Cray's high-performance, 3D torus Gemini network, providing higher bandwidth, lower latency, faster collectives, and greater reliability than the previous generation interconnect.

Titan users will have access to the existing Lustre file systems as well as a next generation Lustre file system with 32 PB of capacity and 1 TB/second of bandwidth. The users will also have access to the HPSS data archive, LENS data analysis and visualization cluster, and the newly upgraded EVEREST high-resolution visualization facility. All of these resources are available through high performance networks including ESnet's recently upgraded 100 gigabit per second links.

Titan System Configuration:

Architecture	Cray XK7
Node	16-Core AMD 6274 Opteron + NVIDIA K20x (Kepler)
Compute Nodes	18,688 hybrid nodes
Compute Node Configuration	16 x86_64 cores + 14 GPU
Aggregate Configuration	299,008 x86 Cores
Memory/Node	32 GB x86 + 6 GB K20x
Memory/Core	2 GB x86
Interconnect	Gemini
GPUs	18,688 K20x Keplers
Speed	27 PF

Mira

Mira, an IBM Blue Gene/Q supercomputer at the Argonne Leadership Computing Facility, is equipped with 786,432 cores, 768 terabytes of memory and has a peak performance of 10 PFLOPS. Mira's 49,152 compute nodes have a PowerPC A2 1600 MHz processor containing 16 cores, each with 4 hardware threads, running at 1.6 GHz, and 16 gigabytes of DDR3 memory. A 17th core is available for the communication library.

IBM's innovative 5D torus interconnect configuration, with 2GB/s chip-to-chip links, connects the nodes, enabling highly efficient computation by reducing the average number of hops and latency between compute nodes. The supercomputer also features a quad floating point unit (FPU) that can be used to execute scalar floating point instructions, four-wide SIMD instructions, or two-wide complex arithmetic SIMD instructions. This quad FPU provides higher single thread performance for some applications.

Mira users have access to a GPFS file system with 24 PB of capacity and 240 GB/second bandwidth. Users also have access to the HPSS data archive and Tukey, the new analysis and visualization cluster. All of these resources are available through high performance networks including ESnet's recently upgraded 100 gigabit per second links.

Mira System Configuration:

Architecture	IBM BG/Q
Node	16-Core PowerPC A2
Compute Nodes	49,152
Compute Node Configuration	16 PPC64 Cores
Aggregate Configuration	786,432 PPC64 Cores
Memory/Node	16 GB RAM per node
Memory/Core	1 GB
Interconnect	5D Torus
GPUs	None
Speed	10 PF

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CONTACTS
INCITE program manager: **incite@doeleadershipcomputing.org**
LCF at Argonne: **incite@alcf.anl.gov**
LCF at Oak Ridge: **help@olcf.ornl.gov**

The INCITE program issues an annual call for proposals, typically from mid-April through the end of June, for awards in the following calendar year. Details appear at **www.doeleadershipcomputing.org**

We encourage you to contact the INCITE program manager and the LCF centers if you have questions about the call for proposals, technical details for Mira and Titan, and how your research campaign may align with the mission of the INCITE program. Individuals and teams of researchers from academia, national laboratories, and industry are eligible to apply and awards of one-, two-, or three-years are granted. Researchers outside of the U.S. may apply.

The Proposal Process

The INCITE peer review process involves two steps: 1) assessing the potential impact of the work, and 2) determining of the applicant's ability to use the Titan and Mira systems.

INCITE and the LCFs offer webinars to advise potential investigators on best practices for INCITE proposal writing. Principal investigators and their teams are encouraged to attend the webinars and to apply for LCF Director's Discretionary (DD) time. DD requests can be submitted at any time and be used to obtain benchmarking data in preparation for the INCITE call for proposals.

The list of questions our reviewers use to assess INCITE proposals are available on the proposal web site and can be helpful for guiding the development of your INCITE application.

The INCITE call for proposals opens in mid-April and closes two and a half months later. A timeline is provided below with suggested activities that may help you better prepare for and respond to the call. DD requests and responses to the INCITE Request for Information (RFI) may be done any time; we suggest they be done early in the year.

1 January/February
Request DD time on Mira or Titan for benchmarking and respond to the INCITE RFI (both optional)

2 April
INCITE Call for Proposals opens

3 April/May
Attend one of the INCITE Proposal Writing Webinars (optional)

4 Late June/Early July
INCITE Call for Proposals closes

5 November
Award notifications are issued

6 January
New INCITE projects begin