INCITE in the International Research Community
May 2014

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Agenda

- History of LCF and INCITE
- INCITE statistics and information
- Sampling of INCITE science and engineering
- How you can become involved
The Secretary of Energy, acting through the Office of Science, shall:

- Establish and operate Leadership Systems Facilities
- Provide access [to Leadership Systems Facilities] on a competitive, merit-reviewed basis to researchers in U.S. industry, institutions of higher education, national laboratories and other Federal agencies
Three primary ways for access to LCF
Distribution of allocable hours

- **60% INCITE**
  5.8 billion core-hours in CY2014

- **Up to 30% ASCR Leadership Computing Challenge**

- **DOE/SC capability computing**

- **10% Director’s Discretionary**

Leadership-class computing
"We are launching the INCITE initiative for two reasons," Dr. Orbach explained. "For one, it's the right thing to do: there are opportunities for major accomplishments in this field of science. In addition, there is also a 'sociology' that we need to develop. We need to learn how to function at those speeds, how to work together as teams, and how to handle and manipulate data.

We want to develop the community of researchers within the United States – and frankly around the world – that can take advantage of these machines and produce the results that will invigorate and revolutionize their fields of study."

Dr. Raymond L. Orbach, Director of DOE's Office of Science
2004 INCITE Call for Proposals
August 1, 2003
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 Facility (LCF) centers for computationally intensive, large-scale research projects.
## INCITE systems: Titan and Mira

<table>
<thead>
<tr>
<th></th>
<th>INCITE Production Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Cray XK7 “Titan”</strong></td>
</tr>
<tr>
<td>Node</td>
<td>16-Core AMD 6274 Opteron + NVIDIA K20x (Kepler)</td>
</tr>
<tr>
<td>Compute Nodes</td>
<td>18,688 hybrid nodes</td>
</tr>
<tr>
<td>Compute Node config</td>
<td>16 x86_64 cores + 14 GPU</td>
</tr>
<tr>
<td>Aggregate Config</td>
<td>299,008 x86 Cores</td>
</tr>
<tr>
<td>Memory/Node</td>
<td>32 GB x86 + 6 GB K20x</td>
</tr>
<tr>
<td>Memory/Core</td>
<td>2 GB x86</td>
</tr>
<tr>
<td>Interconnect</td>
<td>Gemini</td>
</tr>
<tr>
<td>GPUs</td>
<td>18,688 K20x Keplers</td>
</tr>
<tr>
<td>Speed</td>
<td>27 PF</td>
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</table>
Is INCITE right for you?

<table>
<thead>
<tr>
<th>Selecting an allocation program</th>
<th>INCITE</th>
<th>Other</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eligible <em>regardless</em> of funding source or nationality</td>
<td>✔️</td>
<td>?</td>
</tr>
<tr>
<td>Require <em>tens of thousands</em> of cores for production jobs</td>
<td>✔️</td>
<td>?</td>
</tr>
<tr>
<td>Require up to <em>hundreds of millions</em> of core-hours for campaign</td>
<td>✔️</td>
<td>?</td>
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</table>
INCITE breakthroughs since inception
A few of the many science and engineering advances

**Hours requested vs. allocated:**

- ~2X per year
- ~3X per year

<table>
<thead>
<tr>
<th>Hours allocated</th>
<th>4.9 M</th>
<th>6.5 M</th>
<th>18.2 M</th>
<th>95 M</th>
<th>268 M</th>
<th>889 M</th>
<th>1.6 B</th>
<th>1.7 B</th>
<th>1.7 B</th>
<th>4.7 B</th>
<th>5.8 B</th>
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<tbody>
<tr>
<td>Projects</td>
<td>3</td>
<td>3</td>
<td>15</td>
<td>45</td>
<td>55</td>
<td>66</td>
<td>69</td>
<td>57</td>
<td>60</td>
<td>61</td>
<td>59</td>
</tr>
</tbody>
</table>

- **2004**

- **2005**

- **2006**

- **2007**

- **2008**

- **2009**
  - Unprecedented simulation of magnitude-8 earthquake over 125-square miles, *Proceedings, SC10*

- **2010**
  - OMEN breaks the petascale barrier using more than 220,000 cores, *Proceedings SC10*

- **2011**
  - Recovery from slow inactivation in potassium channels controlled by H₂O. *Nature* (2013)

- **2012**
  - NIST proposes new standard reference materials from LCF concrete simulations

- **2013**

- **2014**
INCITE awards and international participation historically

Number of INCITE awards that included at least one non-US-based researcher as PI or co-PI (bar chart)
## INCITE criteria
Access on a competitive, merit-reviewed basis

<table>
<thead>
<tr>
<th></th>
<th>Merit criterion</th>
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<tr>
<td>1</td>
<td>Potential for substantial domain and/or community impact</td>
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</table>

<table>
<thead>
<tr>
<th></th>
<th>Computational leadership criterion</th>
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<tbody>
<tr>
<td>2</td>
<td>Computationally intensive runs that cannot be done anywhere else: capability, architectural needs</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Eligibility criterion</th>
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<tbody>
<tr>
<td>3</td>
<td>Grant allocations regardless of funding source*</td>
</tr>
<tr>
<td></td>
<td>Non-US-based researchers are welcome to apply</td>
</tr>
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</table>
2014 INCITE Peer-Review Panels

Ninety-one participants in the 2014 review

45% participated in the 2013 INCITE review and more than 60% of the reviewers are:

- Society Fellows (APS, IEEE, European Academy of Sciences, AIAA, etc),
- National Academy members,
- Laboratory Fellows
2014 INCITE award statistics

- Request for Information helped attract new projects
- Call closed June 28th, 2013
- Total requests ~14 billion core-hours
- Awards of 5.8 billion core-hours for CY 2014
- 59 projects awarded of which 21 are renewals

Acceptance rates
36% of nonrenewal submittals and 91% of renewals

PIs by Affiliation (Awards)
- US Academia 46%
- US Government 37%
- International 12%
- Industry 5%

Contact information
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whitejc@DOEleadershipcomputing.org
## 2014 award statistics, by system

<table>
<thead>
<tr>
<th></th>
<th>Titan</th>
<th>Mira</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number projects*</td>
<td>30</td>
<td>40</td>
</tr>
<tr>
<td>Average Project</td>
<td>77.6M</td>
<td>88.2M</td>
</tr>
<tr>
<td>Median Project</td>
<td>75M</td>
<td>77.5M</td>
</tr>
<tr>
<td>Total Awards (core-hrs in CY2014)</td>
<td>2.25B</td>
<td>3.53B</td>
</tr>
</tbody>
</table>

* Total of 59 INCITE projects (many of the projects received time on both Mira and Titan)
New PI’s in INCITE

• A “new” PI has never previously led an INCITE submittal
• **34%** of the nonrenewal projects are led by new PI’s
  – 38 new projects awarded, 13 led by new PI’s
INCITE seeks high-impact research campaigns

Examples of previous successful INCITE applications that advance the state of the art across a broad range of topics

- Glimpse into dark matter
- Supernovae ignition
- Protein structure
- Creation of biofuels
- Replicating enzyme functions
- Global climate
- Accelerator design
- Carbon sequestration
- Turbulent flow
- Propulsion systems

- Membrane channels
- Protein folding
- Chemical catalyst design
- Plasma physics
- Algorithm development
- Nano-devices
- Batteries
- Solar cells
- Reactor design
- Nuclear structure
SUMMARY

• 16 km global model in operations today
• 10 km global model planned for 2015, with operational 0-day forecasts to run in less than 1 hour wall time
• 5 km global model is the next target

IMPACT
10 km global IFS model significantly exceeds operational performance requirements for a 2015 implementation.

GPU port is essential to getting the 5 km global IFS model to run operationally in less than one hour; this work will start in 2014. The 5km global IFS Earth-system model has shown great potential in the simulation of rare events such as hurricane Sandy.
DNS of Forced- and Auto-Ignition in Spherical and Engine-Like Geometries
100 million core-hours Christos Frouzakis (Swiss Federal Institute of Technology Zurich)

SUMMARY
Researchers are performing large-scale direct numerical simulations of forced and compression ignition in spherical and engine-like geometries to study the initiation and long-term propagation of premixed flames.

IMPACT
Results will help advance the development of novel combustion systems, such as low-temperature combustion for automobiles and lean premixed combustion for turbine power plants.

The findings will also help to identify the shortcomings of existing engineering models and foster the development of new models.
SUMMARY
Researchers are developing models for turbulent premixed flames to study accidental gas explosions in buildings. With previous INCITE allocations, the team used large eddy simulations to create a unique experimental database, opening the door for researchers to check the validity of models over a range of scales previously not accessible.

IMPACT
This research will help develop a better understanding of the mechanisms controlling explosions in confined spaces, which will feed into the design of safer buildings.

The project is also driving new experiments that are helping to expand the scope of turbulent combustion research.
#1. Key questions to ask yourself

- Is both the scale of the runs and the time demands of the problem of LCF scale?
  - Yes, I can’t get the amount of time I need anywhere else.
  - Yes, my simulations are too large to run on other systems.

- Do you need specific LCF hardware?
  - Yes, the memory and I/O available here are necessary for my work.
#2. Request a start up account now

- Director’s Discretionary Proposals considered year-round
- Award up to millions of hours
- Allocated by LCF center directors

- Director’s Discretionary (DD) requests can be submitted anytime
- DD may be used for porting, tuning, scaling in preparation for an INCITE submittal
- Don’t wait to apply

Argonne DD Program:
http://www.alcf.anl.gov/getting-started/apply-for-dd

Oak Ridge DD Program:
www.olcf.ornl.gov/support/getting-started/olcf-director-discretion-project-application/
#3. Get involved and learn more about us

- Reply to the Request for Information
- Attend an INCITE proposal writing webinar
- Sign up for on-site or virtual meetings at LCF
- Volunteer as a peer-reviewer

Call/email/skype the centers or email INCITE program manager if you’d like an introduction to center managers or staff
#4. Examine resource material

**INCITE General Information**
www.doeleadershipcomputing.org/

**INCITE Proposal Site (includes a sample proposal)**
proposals.doeleadershipcomputing.org/ (see ‘Instructions’)

**INCITE Proposal-Writing Webinar**
http://www.doeleadershipcomputing.org/faqs/ (see ‘Presentations’)

**INCITE Request for Information**
https://proposals.doeleadershipcomputing.org/allocations/incite/
INCITE annual timeline

**Access and Monitoring**

- Jan: Access and monitoring
- Access processing

**Selection and Awards**

- Selection
- Awards

**Solicitation and Review**

- Solicitation (new and renewals)
- Computational Readiness Review
- Panel Peer Review

Timeline:
- Mar
- Apr
- May
- Jun
- Jul
- Aug
- Sept
- Oct
- Nov
- Dec
- Jan
Upcoming activities

Parallel Programming with MPI
Lemont, Illinois
**June 6, 2014**
http://www.alcf.anl.gov/events/parallel-programming-mpi-0

2015 INCITE Call for Proposals Closes
**June 27, 2014**
https://proposals.doeleadershipcomputing.org

2014 OLCF Users Meeting
Oak Ridge, Tennessee
**July 22, 2014 - July 24, 2014**
https://www.olcf.ornl.gov/training-event/2014-olcf-users-meeting/
Contacts

For details about the INCITE program:

- [www.doeleadershipcomputing.org](http://www.doeleadershipcomputing.org) – General information
- [proposals.doeleadershipcomputing.org](http://proposals.doeleadershipcomputing.org) – Proposal site
- INCITE@DOEleadershipcomputing.org

For details about the centers:

- [www.olcf.ornl.gov](http://www.olcf.ornl.gov)
  - [help@nccs.gov](mailto:help@nccs.gov), 865-241-6536

- [www.alcf.anl.gov](http://www.alcf.anl.gov)
  - [support@alcf.anl.gov](mailto:support@alcf.anl.gov), 866-508-9181
Innovative and Novel Computational Impact on Theory and Experiment

INCITE is an annual, peer-review allocation program that provides unprecedented computational and data science resources.

- 5.8 billion core-hours awarded for 2014 on the 27-petaflops Cray XK7 “Titan” and the 10-petaflops IBM BG/Q “Mira”
- Average award: 78 million core-hours on Titan and 88 million core-hours on Mira in 2014
- INCITE is open to any science domain
- INCITE seeks computationally intensive, large-scale research campaigns

Call for Proposals

The INCITE program seeks proposals for high-impact science and technology research challenges that require the power of the leadership-class systems. Allocations will be for calendar year 2015.

April 16 – June 27, 2014

Contact information

Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org
<table>
<thead>
<tr>
<th>Allocation Programs at the LCFs</th>
<th>INCITE</th>
<th>ALCC</th>
<th>Director’s Discretionary</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mission</strong></td>
<td>High-risk, high-payoff science that requires LCF-scale resources*</td>
<td>High-risk, high-payoff science aligned with DOE mission</td>
<td>Strategic LCF goals</td>
</tr>
<tr>
<td><strong>Call</strong></td>
<td>1x/year – (Closes June)</td>
<td>1x/year – (Closes February)</td>
<td>Rolling</td>
</tr>
<tr>
<td><strong>Duration</strong></td>
<td>1-3 years, yearly renewal</td>
<td>1 year</td>
<td>3m,6m,1 year</td>
</tr>
<tr>
<td><strong>Typical Size</strong></td>
<td>50 – 70 projects, 50M – 100's M core-hours/yr.</td>
<td>10 – 20 projects, 1M – 75M core-hours/yr.</td>
<td>100s of projects, 10K – 1M core-hours</td>
</tr>
<tr>
<td><strong>Review Process</strong></td>
<td>Scientific Peer-Review, Computational Readiness</td>
<td>Scientific Peer-Review, Computational Readiness</td>
<td>Strategic impact and feasibility</td>
</tr>
<tr>
<td><strong>Managed By</strong></td>
<td>INCITE management committee (ALCF &amp; OLCF)</td>
<td>DOE Office of Science</td>
<td>LCF management</td>
</tr>
<tr>
<td><strong>Availability</strong></td>
<td>Open to all scientific researchers and organizations</td>
<td>Capability &gt;20% of cores</td>
<td></td>
</tr>
</tbody>
</table>
A sample of codes with local expertise available at Argonne and Oak Ridge

<table>
<thead>
<tr>
<th>Application</th>
<th>Field</th>
<th>ALCF</th>
<th>OLCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLASH</td>
<td>Astrophysics</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>MILC,CPS</td>
<td>LQCD</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Nek5000</td>
<td>Nuclear energy</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Rosetta</td>
<td>Protein structure</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>DCA++</td>
<td>Materials science</td>
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<td>ANGFMC</td>
<td>Nuclear structure</td>
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<tr>
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<td>Qbox</td>
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<td>✓</td>
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<tr>
<td>LAMMPS</td>
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<tr>
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<tr>
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<tr>
<td>NAMD</td>
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<table>
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<tr>
<th>Application</th>
<th>Field</th>
<th>ALCF</th>
<th>OLCF</th>
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<tr>
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<td>GTC,GTX</td>
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