U.S. DEPARTMENT OF ENERGY

INCITE

LEADERSHIP COMPUTING

# INCITE Overview

## April 17, 2012

Julia C. White, INCITE Manager

Presentation to OLCF Spring Training and Users Meeting

# US DOE user facilities

- State-of-the art scientific research facilities
- Shared with the science community worldwide
- Offering technologies and instrumentation that are not available elsewhere

# Solving scientific challenges

*"Computation and supercomputing are critical to solving some of our greatest scientific challenges."*

- Steven Chu, U.S. Energy Secretary

*"I look forward to witnessing the promise of these efforts as some of the world's greatest thinking minds use some of the world's greatest thinking computers."*

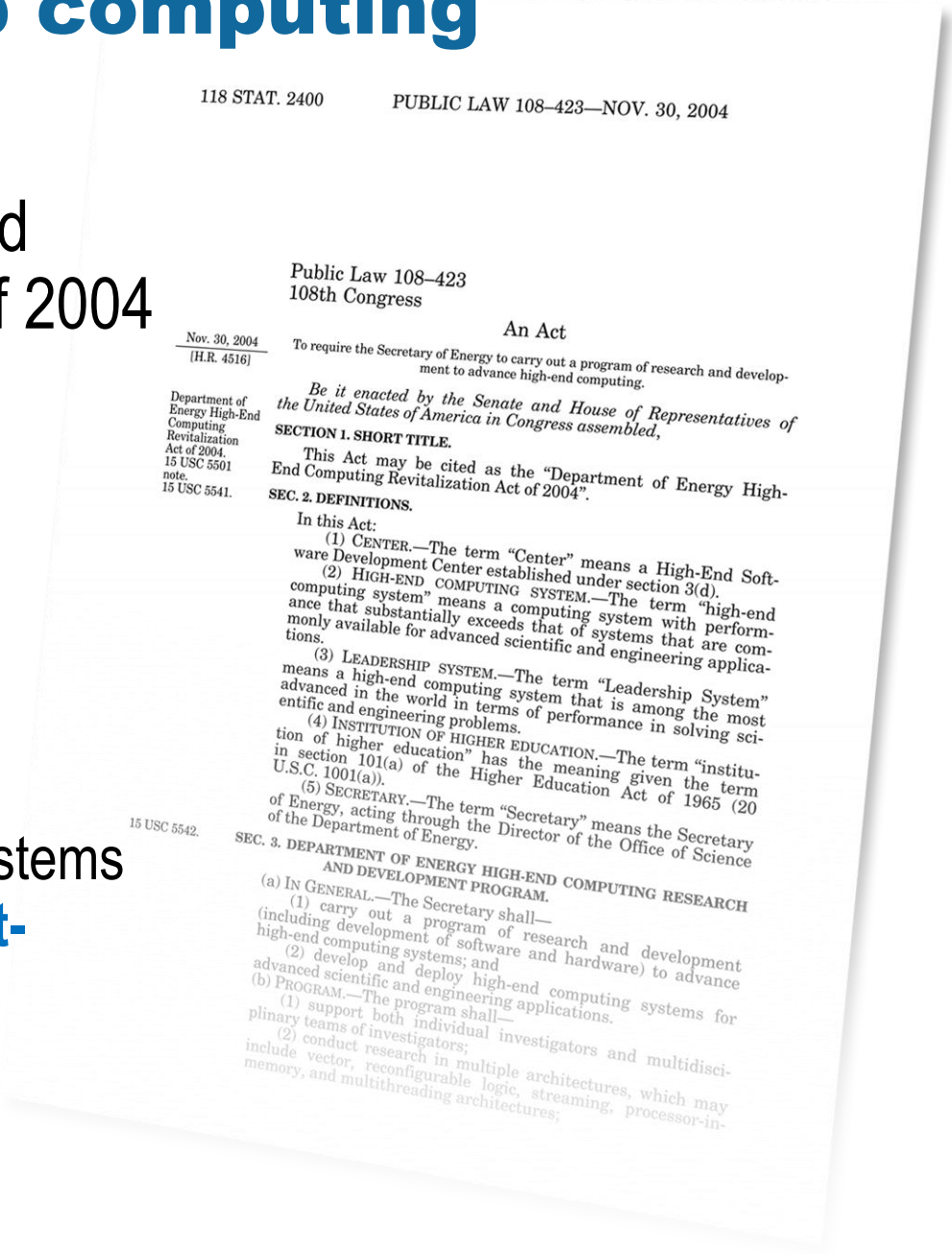
- Samuel Bodman, U.S. Energy Secretary, 2005-2009 on DOE supercomputers

# Origin of leadership computing facilities: LCFs

Department of Energy High-End Computing Revitalization Act of 2004 (Public Law 108-423):

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



118 STAT. 2400 PUBLIC LAW 108–423—NOV. 30, 2004

Public Law 108–423
108th Congress

An Act

Nov. 30, 2004
[H.R. 4516]

To require the Secretary of Energy to carry out a program of research and development to advance high-end computing.

*Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,*

Department of Energy High-End Computing Revitalization Act of 2004. 15 USC 5501 note.

**SECTION 1. SHORT TITLE.**

This Act may be cited as the "Department of Energy High-End Computing Revitalization Act of 2004".

15 USC 5541.

**SEC. 2. DEFINITIONS.**

In this Act:

(1) CENTER.—The term "Center" means a High-End Software Development Center established under section 3(d).

(2) HIGH-END COMPUTING SYSTEM.—The term "high-end computing system" means a computing system with performance that substantially exceeds that of systems that are commonly available for advanced scientific and engineering applications.

(3) LEADERSHIP SYSTEM.—The term "Leadership System" means a high-end computing system that is among the most advanced in the world in terms of performance in solving scientific and engineering problems.

(4) INSTITUTION OF HIGHER EDUCATION.—The term "institution of higher education" has the meaning given the term in section 101(a) of the Higher Education Act of 1965 (20 U.S.C. 1001(a)).

(5) SECRETARY.—The term "Secretary" means the Secretary of Energy, acting through the Director of the Office of Science of the Department of Energy.

15 USC 5542.

**SEC. 3. DEPARTMENT OF ENERGY HIGH-END COMPUTING RESEARCH AND DEVELOPMENT PROGRAM.**

(a) IN GENERAL.—The Secretary shall—

(1) carry out a program of research and development (including development of software and hardware) to advance high-end computing systems; and

(2) develop and deploy high-end computing systems for advanced scientific and engineering applications.

(b) PROGRAM.—The program shall—

(1) support both individual investigators and multidisciplinary teams of investigators;

(2) conduct research in multiple architectures, which may include vector, reconfigurable logic, streaming, processor-in-memory, and multithreading architectures;

# Establish and operate leadership computing facilities

**Top500 List (Nov 2011)**

**#3** Cray XT "Jaguar" at the Oak Ridge Leadership Computing Facility (OLCF)

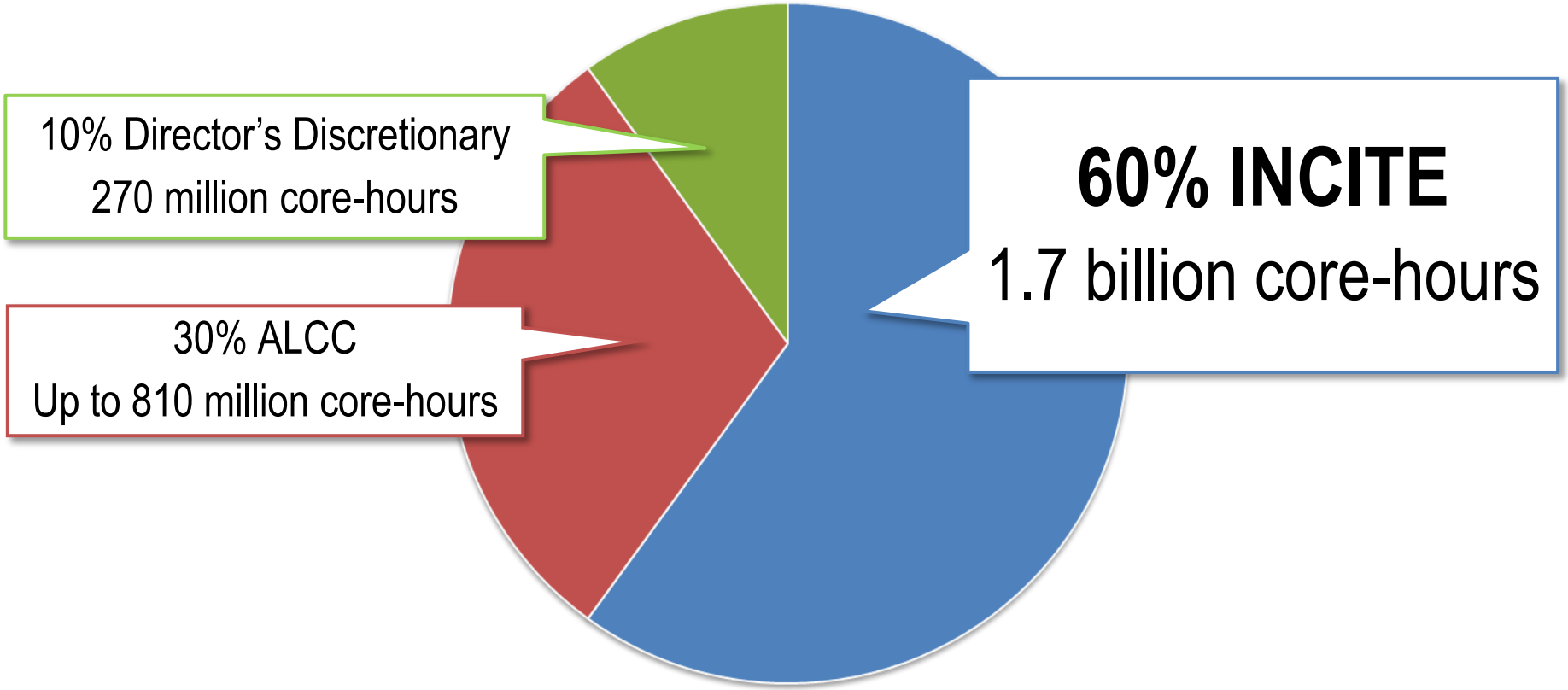
**#23** IBM BG/P "Intrepid" at the Argonne Leadership Computing Facility (ALCF)

*Both LCFs are carrying out system upgrades, to be completed in 2013*

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

# Provide access to LCFs:
## More than 2.7 billion core hours awarded in 2012



# Allocation Programs at the LCFs

| | INCITE (60%) | | ALCC (30%) | | Director's Discretionary (10%) | |
|---|---|---|---|---|---|---|
| **Mission** | High-risk, high-payoff science that requires LCF-scale resources* | | High-risk, high-payoff science aligned with DOE mission | | Strategic LCF goals | |
| **Call** | 1x/year – (Closes June) | | 1x/year – (Closes February) | | Rolling | |
| **Duration** | 1-3 years, yearly renewal | | 1 year | | 3m,6m,1 year | |
| **Typical Size** | 30 - 40 projects | 10M - 100M core-hours/yr. | 5 - 10 projects | 1M – 75M core-hours/yr. | 100s of projects | 10K – 1M core-hours |
| **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 | |
| **Availability** | Open to all scientific researchers and organizations<br>*Capability >20% of cores* | | | | | |

# Is INCITE right for me?

INCITE seeks computationally intensive, large-scale research projects with the potential to significantly advance key areas in science and engineering.

**1 Impact criterion**

High-impact science and engineering

**2 Computational leadership criterion**

Computationally intensive runs that cannot be done anywhere else

**3 Eligibility criterion**

- INCITE grants allocations **regardless of funding source** (ex. DOE, NSF, private, etc)
- **Non-US-based researchers** are welcome to apply

**Call for 2013 proposals opens in Spring 2012**

The INCITE program seeks proposals for high-impact science and technology research challenges that require the power of the leadership-class systems

# Twofold review process

| | New proposal assessment | Renewal assessment |
|---|---|---|
| 1 Peer review: INCITE panels | • **Scientific and/or technical merit**<br>• Appropriateness of proposal method, milestones given<br>• Team qualifications<br>• Reasonableness of requested resources | • Change in scope<br>• **Met milestones**<br>• On track to meet future milestones<br>• **Scientific and/or technical merit** |
| 2 **Computational readiness review: LCF centers** | • Technical readiness<br>• Appropriateness for requested resources | • Met technical/ computational milestones<br>• On track to meet future milestones |
| **Award Decisions** | • INCITE Awards Committee comprised of LCF directors, INCITE program manager, LCF directors of science, sr. management | |

# INCITE awards history

*20X growth in number of projects*

**… but 1000X growth in hours**

| | 2004 | 2005 | 2006 | 2007 | 2008 | 2009 | 2010 | 2011 | 2012 | 2013 |
|---|---|---|---|---|---|---|---|---|---|---|
| Projects | 3 | 3 | 15 | 45 | 55 | 66 | 69 | 57 | 60 | *TBD* |
| Hours allocated | 4.9M | 6.5M | 18.2M | 95M | 268M | 889M | 1.6B | 1.7B | 1.7B | ***5B*** |

NERSC: 3 projects and 4.9M hours awarded

ALCF, OLCF, PNNL join INCITE

INCITE management by ALCF and OLCF; PNNL and NERSC transition out at end of 2009*

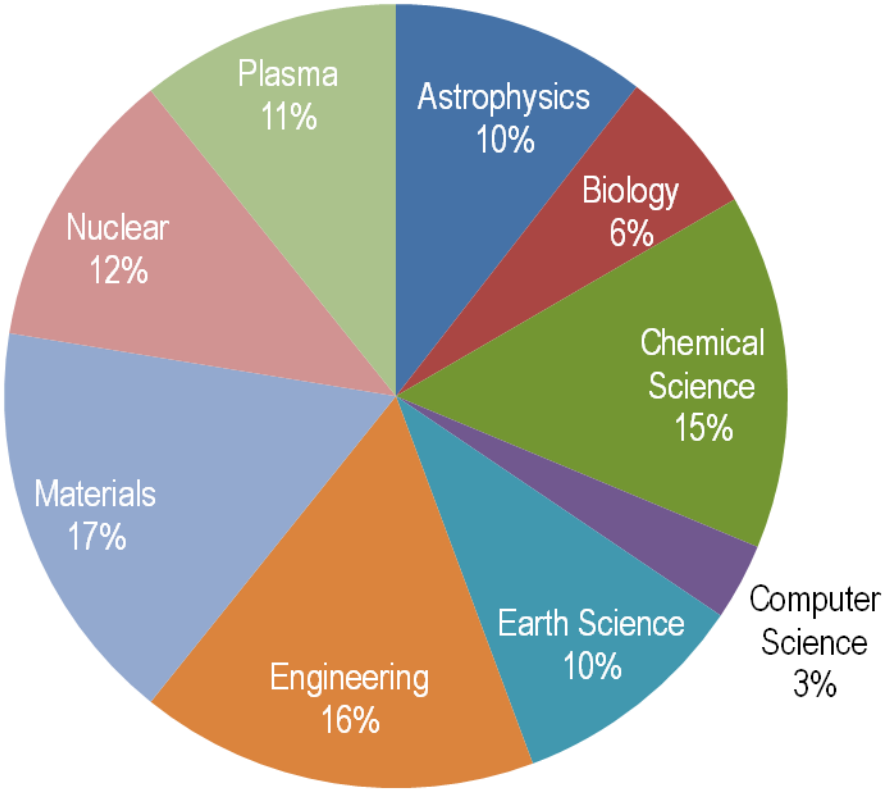
*ALCF and OLCF: Mira and Titan*

# 2012 INCITE allocations

## 28 new projects, 32 renewals

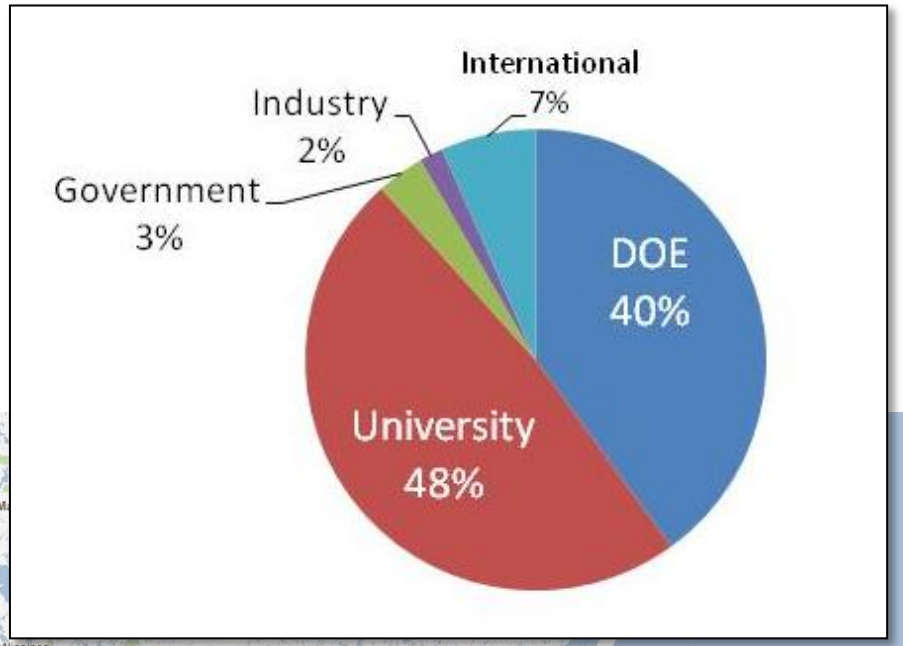
## Acceptance rate: 33% for new proposals, 91% for renewals

Distribution of INCITE time by science domain



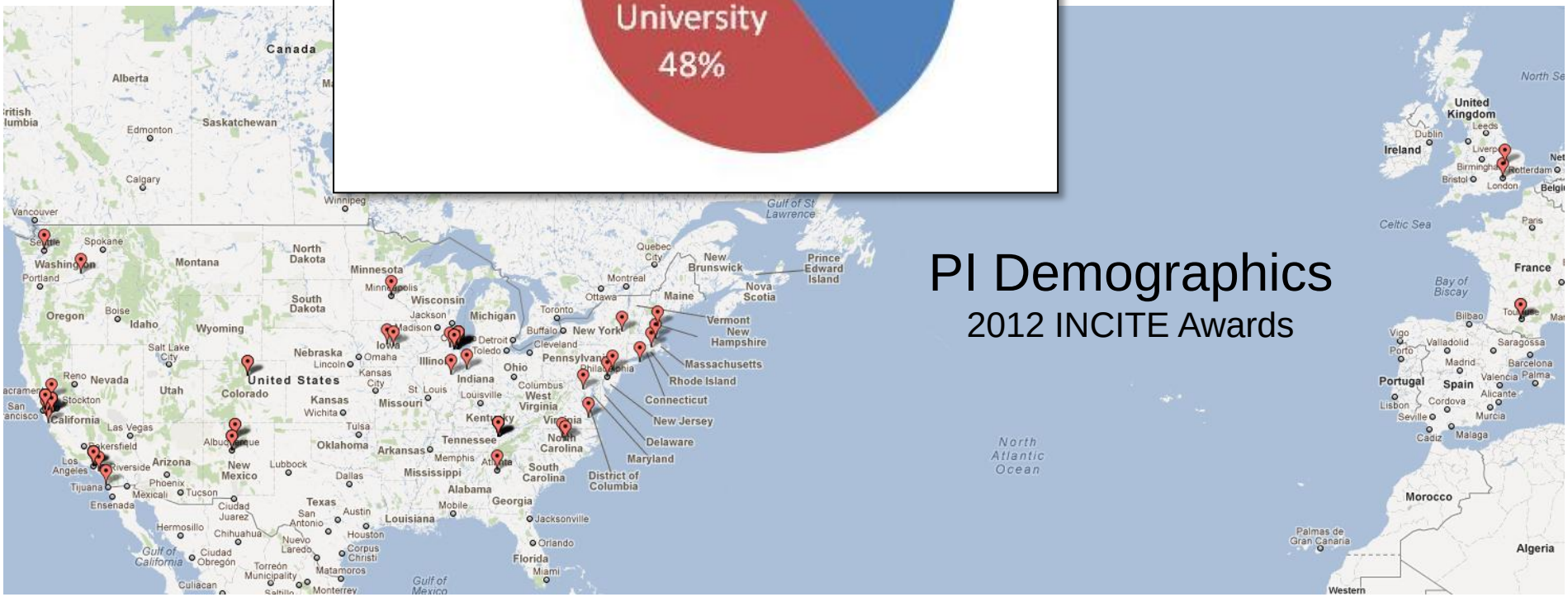

**Awarded 1.67 billion hours for CY 2012**

# 2012 INCITE award demographics




PI Affiliations

2012 INCITE Awards

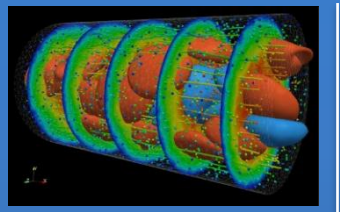



PI Demographics

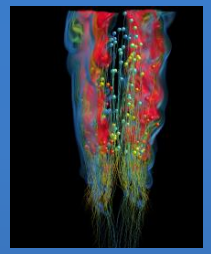
2012 INCITE Awards

# Diversity of INCITE science

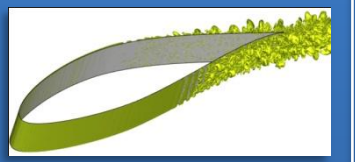
Simulating a flow of healthy (red) and diseased (blue) blood cells with a Dissipative Particle Dynamics method.
*- George Karniadakis, Brown University*



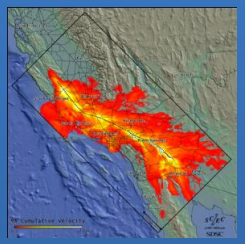
Provide new insights into the dynamics of turbulent combustion processes in internal-combustion engines.
*-Jacqueline Chen and Joseph Oefelein, Sandia National Laboratories*



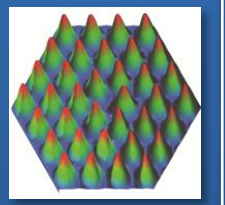
Demonstration of high-fidelity capture of airfoil boundary layer, an example of how this modeling capability can transform product development.
*- Umesh Paliath, GE Global Research*



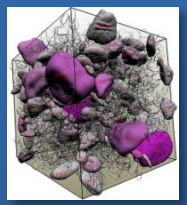
Calculating an improved probabilistic seismic hazard forecast for California.
*- Thomas Jordan, University of Southern California*



Modeling charge carriers in metals and semiconductors to understand the nature of these ubiquitous electronic devices.
*- Richard Needs, University of Cambridge, UK*



High-fidelity simulation of complex suspension flow for practical rheometry.
*- William George, National Institute of Standards and Technology*



## Other INCITE research topics

- Glimpse into dark matter
- Supernovae ignition
- Protein structure
- Creation of biofuels
- Replicating enzyme functions
- Global climate
- Regional earthquakes
- Carbon sequestration
- Turbulent flow
- Propulsor systems
- Membrane channels
- Protein folding
- Chemical catalyst design
- Combustion
- Algorithm development
- Nano-devices
- Batteries
- Solar cells
- Reactor design
- Nuclear structure

# 2013 INCITE Call for Proposals

**More than 5 billion core-hours will be allocated for Calendar Year 2013**

## What's new

- Guidelines about ensemble simulations and the capability metric
- Management plan required
- Development plan for next-gen system
- Request for Information

## 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 2013.

**April 11 – June 27, 2012**

**Contact information**

Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org

# More about our ensemble policy

## or, "Can I meet the computationally intensive criterion by loosely coupling my jobs?"

- Possibly "yes",
  - If you require large numbers of discrete or loosely coupled simulations where time-to-solution is an untenable pacing issue, **and**
  - If a software workflow solution (e.g., pre- and post-processing scripts that automate run management and analysis) is provided to facilitate this volume of work.
- Probably "no",
  - If by decoupling the simulations the work could be effectively carried out on a smaller resource within a reasonable time-to-solution.

**TIPS** | **Do** examine the Frequently Asked Questions for these and other topics at http://hpc.science.doe.gov/allocations/incite/faq.do

# Management Plan

| | |
|---|---|
| 1 | Principal investigator and co-principal investigators |
| 2 | Project title |
| 3 | Research category |
| 4 | Project summary (50 words) |
| 5 | Computational resources requested |
| 6 | Funding sources |
| 7 | Other high-performance computing support for this project |
| 8 | Project narrative, other materials |
| | (A) executive summary (1 page) |
| | (B) project narrative, including computational readiness, job characterization (15 pages) |
| | (C) personnel justification **and management plan** (1 page) |
| 9 | Application packages |
| 10 | Proprietary and sensitive information |
| 11 | Export control |
| 12 | Monitor information |

# Project Narrative: Next-generation systems

- **LCF resources in CY2013 and CY2014 will have new and highly parallel architectures**
  - Local memory per flop will dramatically decrease
  - Relative cost of data movement to/from accelerators will become a potential bottleneck

**TIPS** | **Do** provide a development plan articulating a strategy for maximizing node-level parallelism.

# Project Narrative: Next-generation systems

- **Strategies to consider**
  - Hybridization utilizing OpenMP or Pthreads to expose thread-level or SMP-like parallelism
  - Exposing vector or streaming parallelism through, e.g. CUDA, OpenCL, compiler directives, etc.
  - Algorithmic improvements or design to maximize data locality and memory hierarchy usage

# Request for Information

We invite prospective INCITE-proposal PIs to respond to a Request for Information to inform the INCITE management of the proposal topics anticipated. The information requested here is **not** a prerequisite for proposal submittal, nor will it limit any requests you may decide to make in your INCITE proposal.

http://hpc.science.doe.gov/allocations/incite/

*The response to date includes expressions of interest from across the US, Europe, and Asia.*

# INCITE's broader impact

*"One of the most important aspects of the INCITE program is that **the resulting knowledge will largely be available**, so that the information and technologies can be used by other researchers, further broadening the impact of this work."*

- DOE Under Secretary for Science Raymond Orbach, 2006-2009, Director of DOE Office of Science 2002-2005, who launched INCITE in 2003.

# Who hears about your work (and why you should care)

| Products | Audience | Result |
| --- | --- | --- |
| Publications<br>Presentations<br>Press releases<br>Quarterly reports | Your research community<br>Your reviewers<br>Your sponsor<br>*and*<br>The LCF sponsor<br>The U.S. government | Your monetary grants, and allocation awards<br>*and*<br>LCF funding for support, upgrades, new systems |

By **acknowledging** the LCF and the INCITE program, you **maximize** the impact of your work and its potential for growth.

# More on acknowledgements

- In the **2014 INCITE Call for Proposals**, we will ask for a list of publications resulting from any previous INCITE award.
- Only those with appropriate acknowledgements will be counted (see INCITE FAQs).

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An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.

and either

This research used resources of the Oak Ridge Leadership Computing Facility located in the Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract DE-AC05-00OR22725.

This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

# A few final words about INCITE

INCITE allocations are among the largest available anywhere and, per project, are **equivalent to <u>millions</u> of US dollars**.

**Scientific support staff** have been assigned to your project, to help you succeed. Take advantage of this.

LCF's are very motivated to **communicate** your project's successes. Stay in touch with them.

# Relevant links

**INCITE Program**
www.doeleadershipcomputing.org/

**Argonne Discretionary Program**
www.alcf.anl.gov/resource-guides/getting-started-directors-discretionary

**Oak Ridge Discretionary Program**
www.olcf.ornl.gov/support/getting-started/olcf-director-discretion-project-application

**Contact the center if you'd like to request Discretionary time for benchmarking**

# Contacts

**For details about the INCITE program:**

www.doeleadershipcomputing.org
INCITE@DOEleadershipcomputing.org

**For details about the centers:**

www.olcf.ornl.gov
help@nccs.gov, 865-241-6536

www.alcf.anl.gov
support@alcf.anl.gov, 866-508-9181