U.S. DEPARTMENT OF ENERGY

INCITE

LEADERSHIP COMPUTING

INCITE Overview

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ASCAC

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What is INCITE?

INCITE: Innovative and Novel Computational Impact on Theory and Experiment

Provides awards to academic, government, and industry organizations worldwide needing large allocations of computer time, supporting resources, and data storage to pursue transformational advances in science and industrial competitiveness.

Beginning in 2010, INCITE is jointly run by the ALCF and OLCF, managed by Julia White

OAK RIDGE National Laboratory

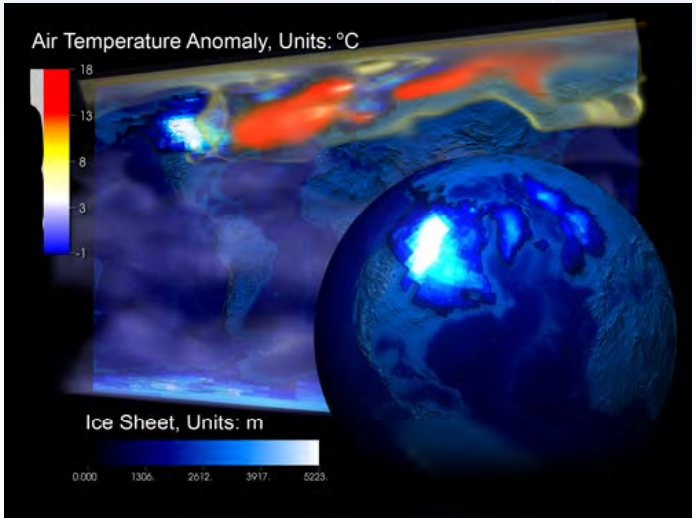
Argonne NATIONAL LABORATORY

INCITE LEADERSHIP COMPUTING

High-resolution climate modeling

Providing accurate scenarios of future climate change

Key challenges	Key benefits	Computing solutions
• Anthropogenic climate change and global warming concerns drive the need to improve the scientific basis for assessing the potential ecological, economic, and social impacts of climate change • The goal of decadal prediction requires long-time integrations of models at unprecedented resolutions	• Predicting and simulating the possibility of abrupt climate change on the timescale of decades rather than centuries • Mitigating deleterious effects of global climate change	• Higher fidelity simulations made possible by petascale computing are improving predictive capability and the ability to realistically represent features such as precipitation patterns and tropical storms



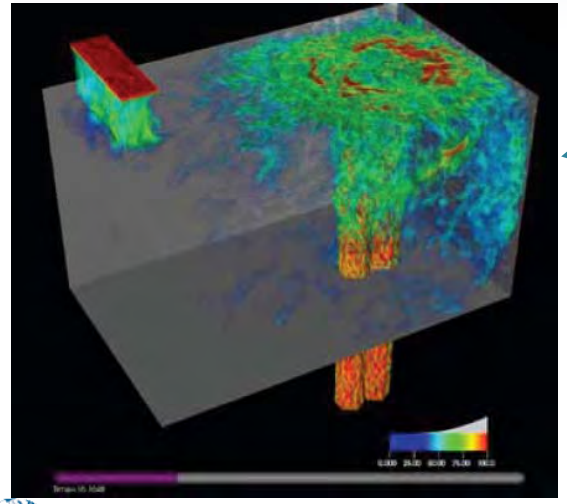
Visualization: Jamison Daniel, ORNL

Abrupt climate change: Running NCAR's CCSM3 model, the simulation shows deglaciation during the Bolling-Allerod, Earth's most recent period of natural global warming

Advances in nuclear reactor modeling

Making safe, clean nuclear energy available globally

Key challenges	Key benefits	Computing solutions
• Developing new technologies that will dramatically expand the availability of safe, clean nuclear energy to help meet the growing global energy demand	• Simulations will enable researchers to gain an understanding of the fundamental thermal mixing phenomena within advanced recycling reactor cores, which can lead to improved safety and economy of these pivotal designs	• Validating the core hydrodynamics large-eddy simulations by comparing highly detailed simulations in similar configurations • Simulations of coolant flow in a simplified geometry to allow resolving all turbulent motion with no model assumptions



"Computations… are already yielding important results in the analysis and understanding of reactor core flows, including establishment of turbulent flow entry lengths and subassembly coolant mixing characteristics."

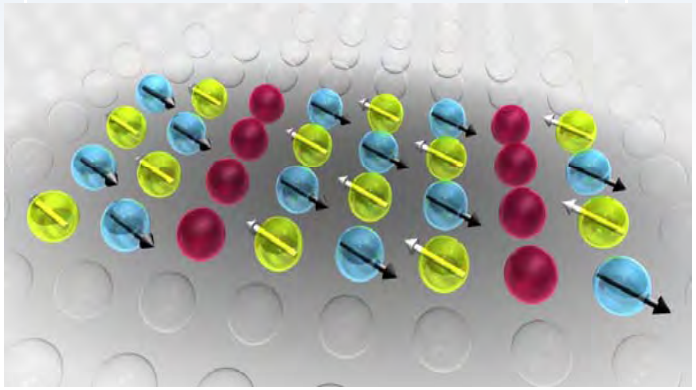
Dr. Paul Fischer, Argonne National Laboratory

Representation of turbulent flow of coolant into a mock-up of the upper plenum of an advanced recycling nuclear reactor. The colors indicate the speed of the fluid.

High-temperature superconductor design

Revolutionary simulations for improved energy transmission

Key challenges	Key benefits	Computing solutions
• Simulations of high-temperature superconductors to provide a deeper understanding of existing materials and the design of new materials with predetermined properties • Application of Hubbard model to understand role of inhomogeneties in cuprates—paving the way for higher temperature superconductors	• Research into the nature of materials promises to revolutionize many areas of modern life, from power generation and transmission to transportation and faster, smaller computers and storage devices	• Petascale simulations are increasing the accuracy and fidelity of superconductivity simulations • Improved understanding will increase nanoscience and nanotechnology capabilities to improve U.S. competitiveness and industrial leadership



Dynamic cluster quantum Monte Carlo simulation of the striped state in the 1/8 doped LaBaCuO high-temperature cuprate superconductor. Consistent with experiments, the simulations show evidence that superconductivity is optimized in this state.

Simulation: Thomas Maier, Gonzalo Alvarez, Mike Summers, ORNL & Thomas Schulthess, ETH Zürich;
Visualization: Jeremy Meredith, ORNL

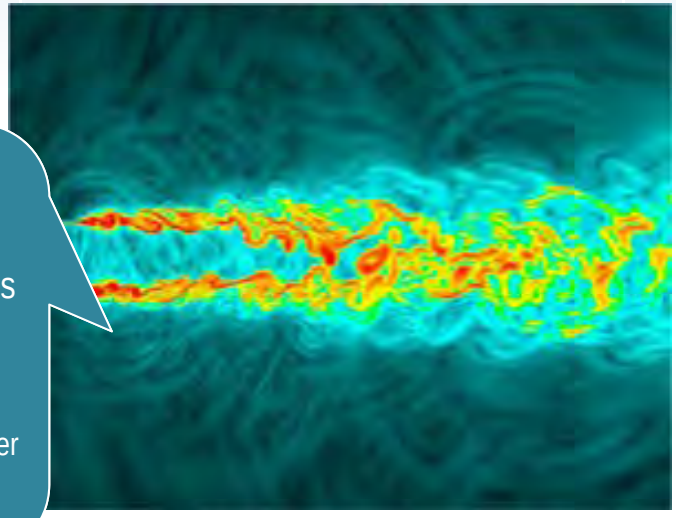
Next-generation energy and propulsion

First proof-of-concept aero and acoustic large-eddy simulation (LES) calculation completed

Key challenges	Key benefits	Computing solutions
• Reduce airfoil trailing edge noise—a key component in wind turbine noise generation • Tackle the yield-limiting noise barrier for wind turbines using simulation-based aeroacoustics via large-scale computing	• Quieter and larger blades and a significant increase in the energy yields possible from the wind portion of the world's renewable portfolio	• Comparisons with available experimental data show that the LES predictions are successful in predicting key flow phenomena

"As this technology develops, it will accelerate GE's ability to design quieter and larger blades and significantly increase the energy yields possible from the wind portion of the world's renewable portfolio."

Dr. Gary Leonard, Global Technology Leader
Energy and Propulsion Technologies
GE Global Research



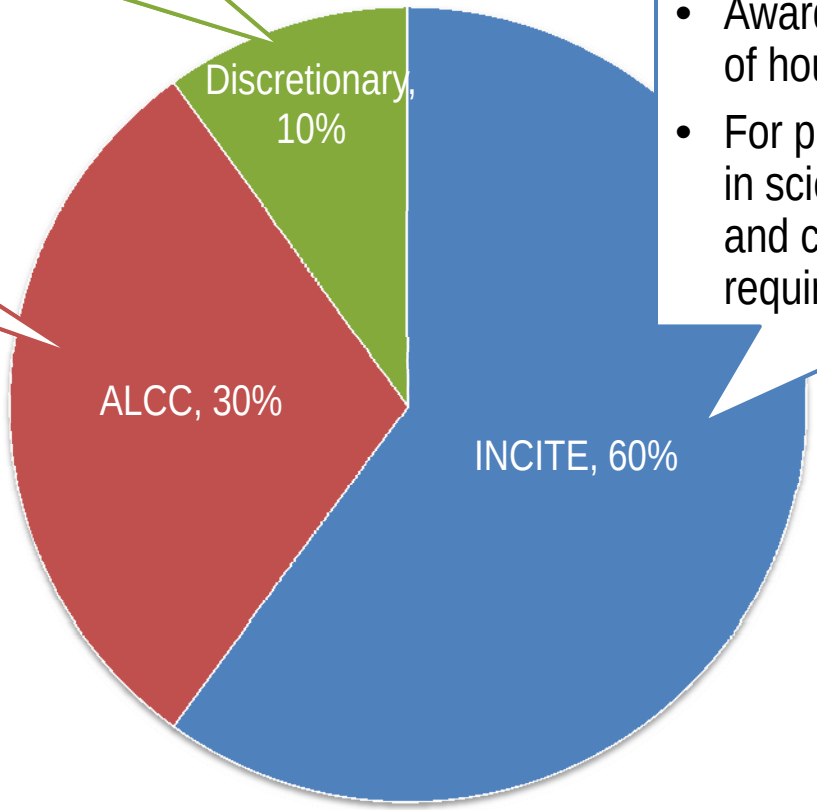
Reducing aerodynamic noise is critical to the viability of next-generation "green" low-carbon/greenhouse gas emission energy systems (e.g., wind turbines)

LCF allocation programs
More than 2.7 billion processor hours

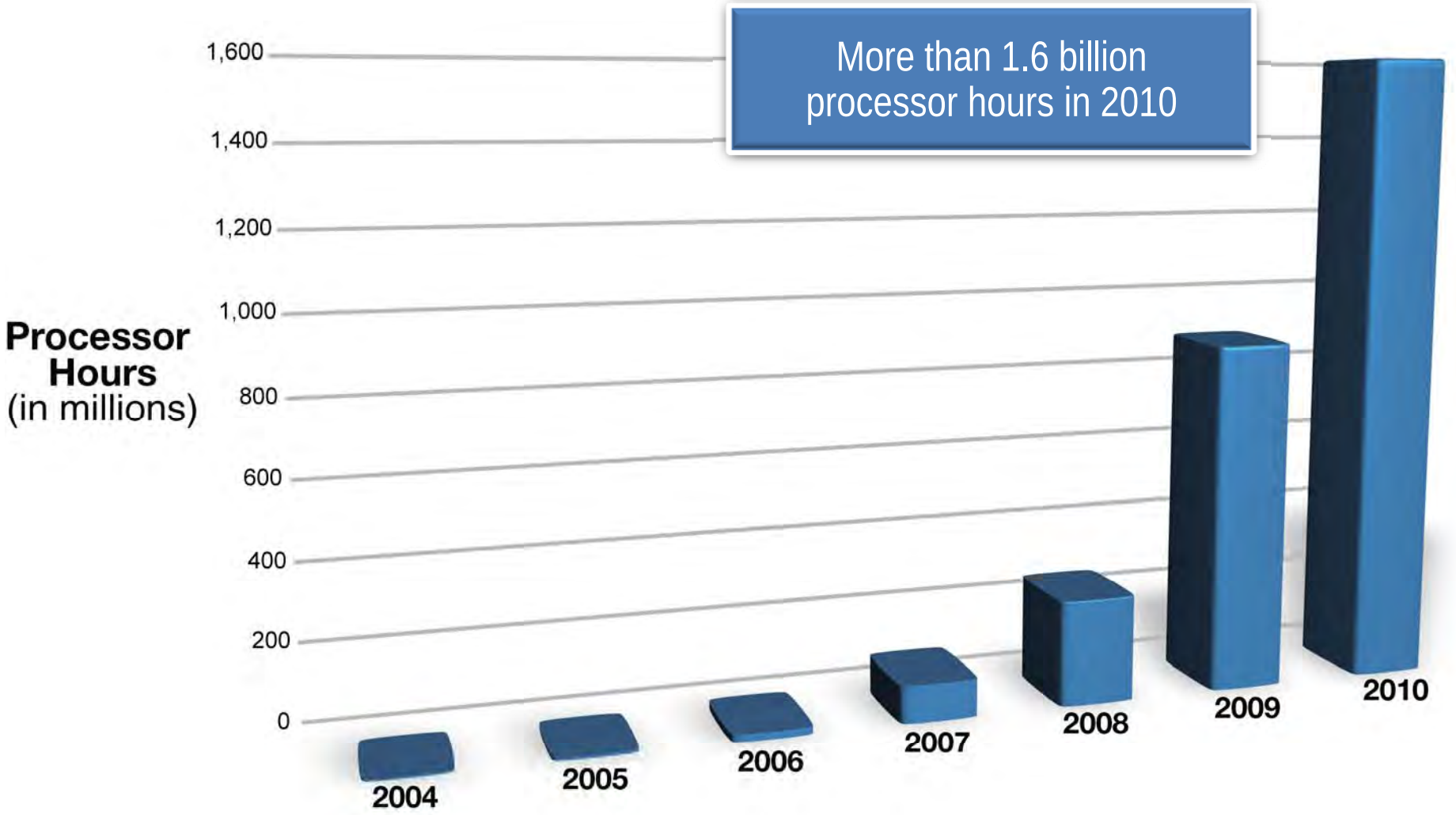
- Proposals considered year-round
- Award up to millions of hours

- Annual call for proposals
- Award tens of millions of hours
- For projects of high impact in science, engineering, and computer science that require leadership systems

- Allocated by the ASCR office



INCITE in its 7th year
Explosive growth in program allocations



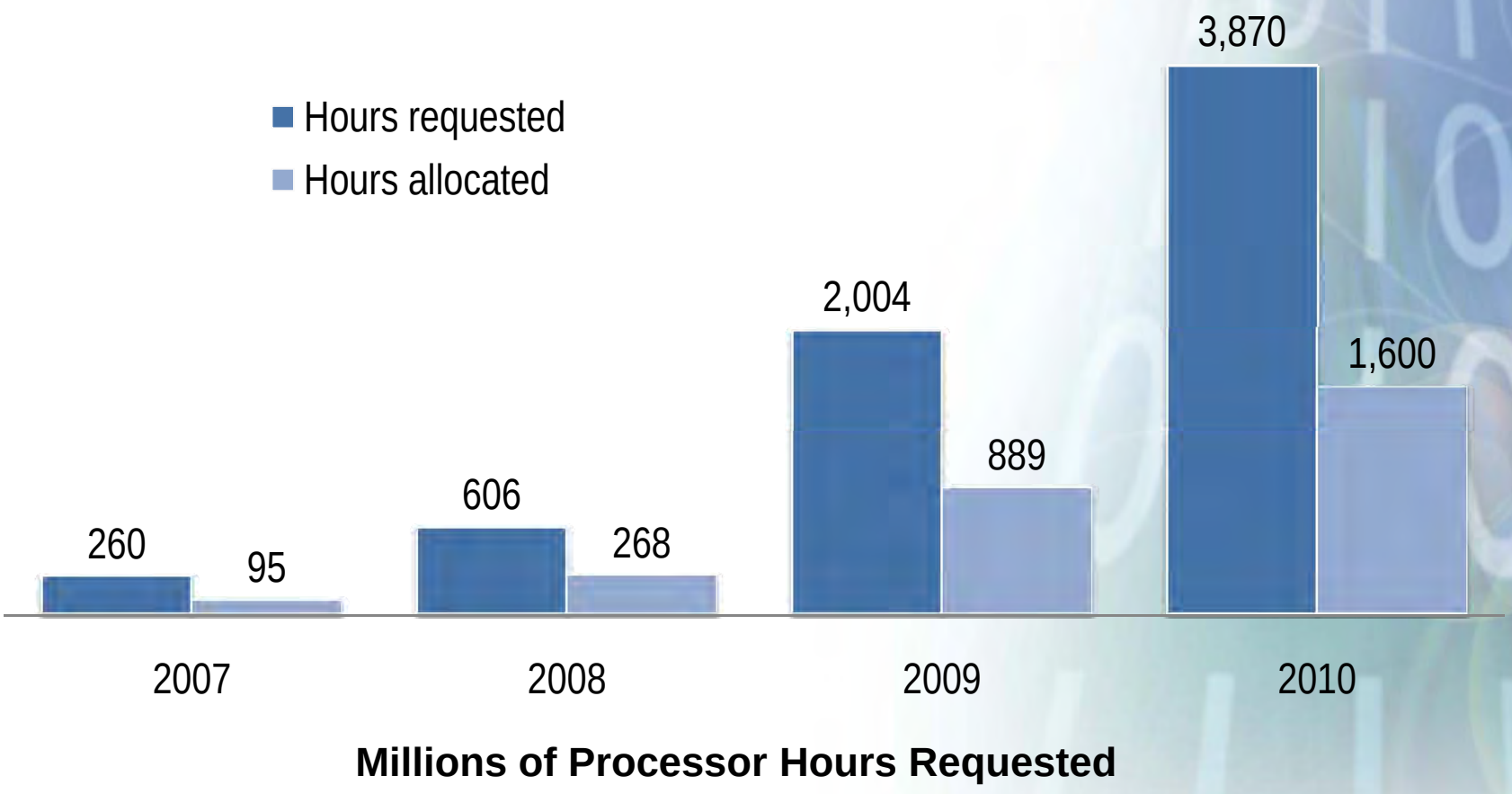
INCITE is open to researchers worldwide from academic, government, and industry organizations

Advancing the state of the art across a range of disciplines

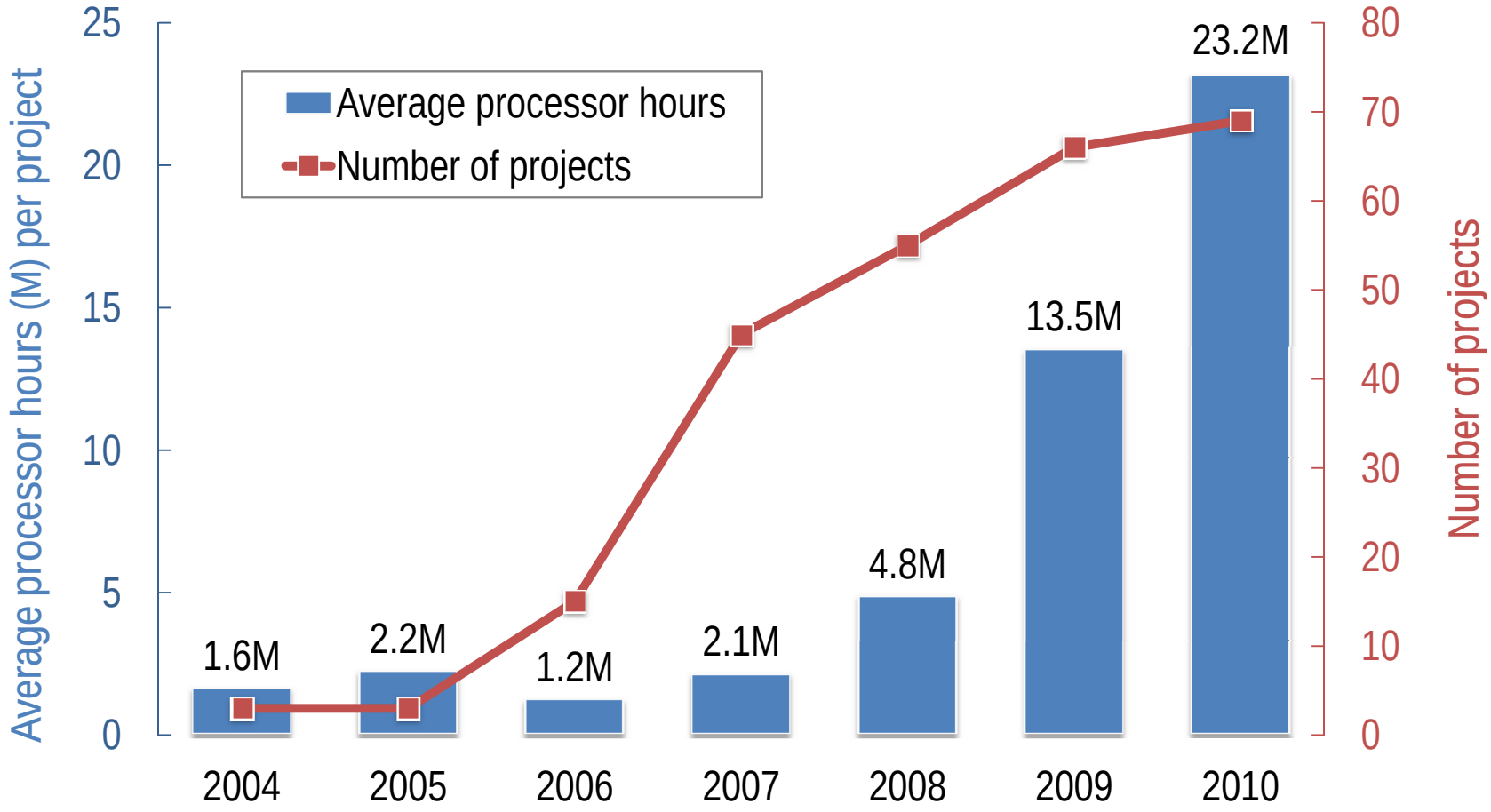
- Accelerator physics
- Astrophysics
- Bioenergy
- Chemical sciences
- Computer Science
- Engineering
- Climate research
- Environmental science
- Life sciences
- Materials science
- Fusion energy
- Nuclear physics

- No designated number of hours for a particular science area
- INCITE looks at all recommendations, focusing on potential for scientific or technological impact, then readiness

The INCITE program is typically 2.5× oversubscribed

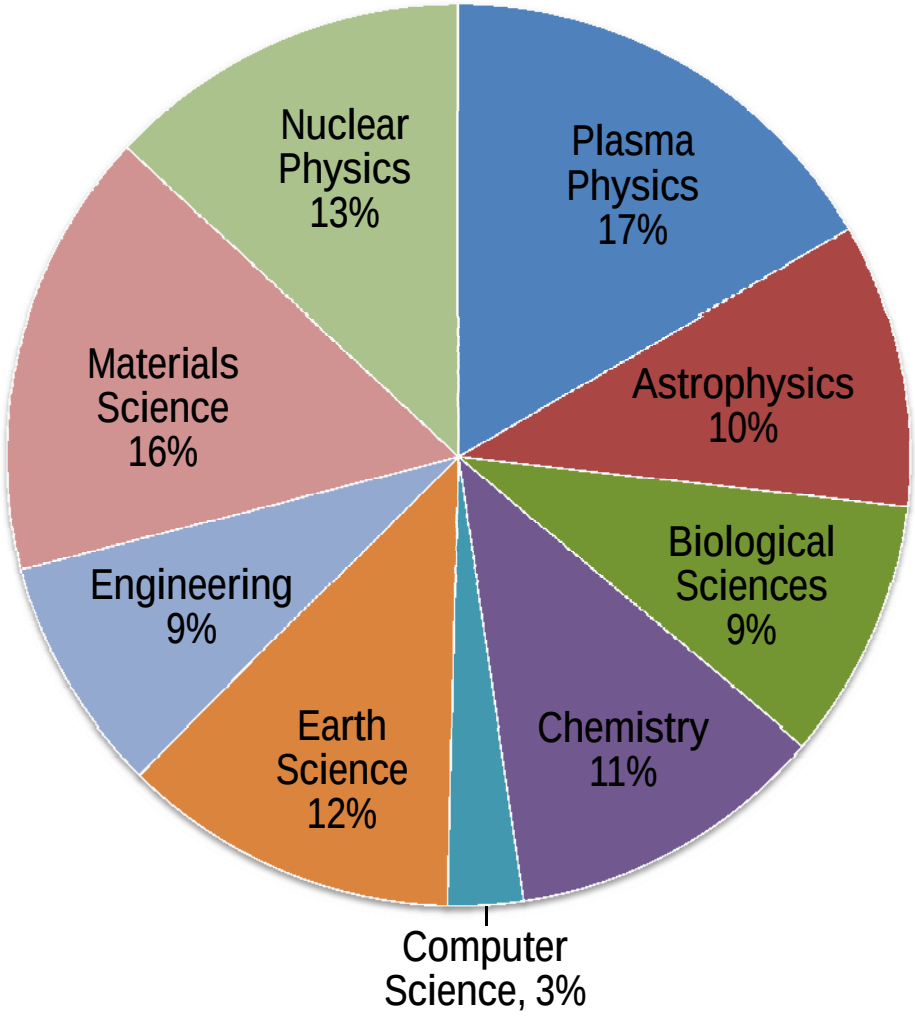


INCITE awards have grown in size and number

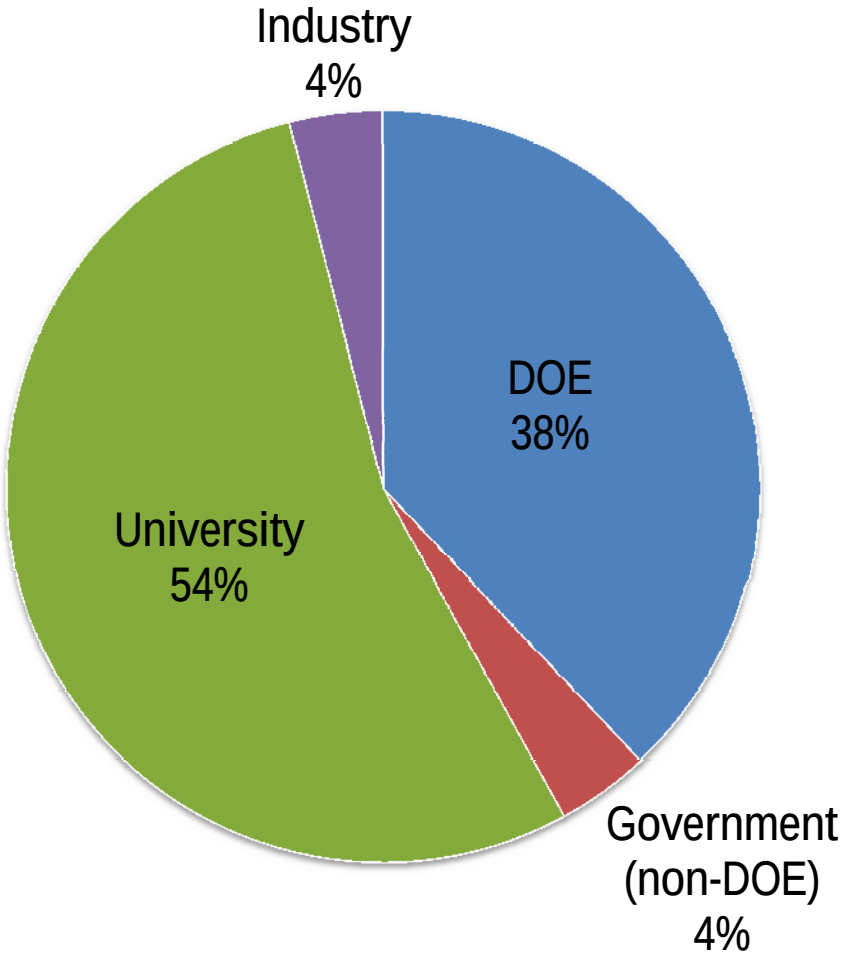


INCITE 2010 awards:

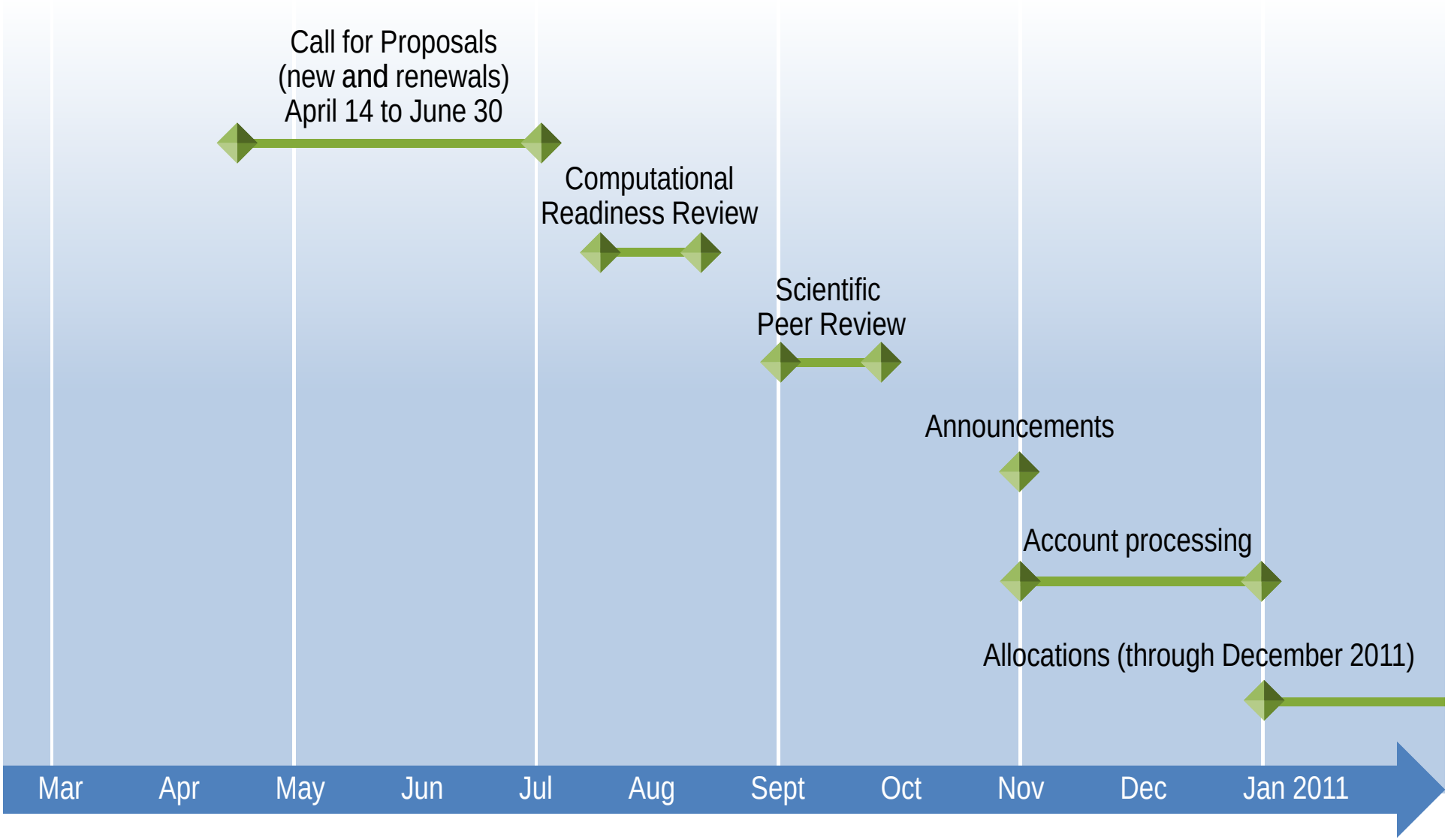
35 new projects and 34 renewal projects
41% of new submittals and 83% of renewals



2010 project demographics by PI affiliation



INCITE 2011: Schedule for proposals



Review process: Computational readiness

- Reviewers: Center staff who are expert in these systems
- Both centers review each proposal

Criteria for new proposals	Criteria for renewals*
• Appropriateness for requested resources • Appropriateness of computational approach • Technical readiness	• Met technical and computational milestones • On track to meet future milestones

*Assessment of renewals, as recommended by 2008 Committee of Visitors

Review process: Panel review

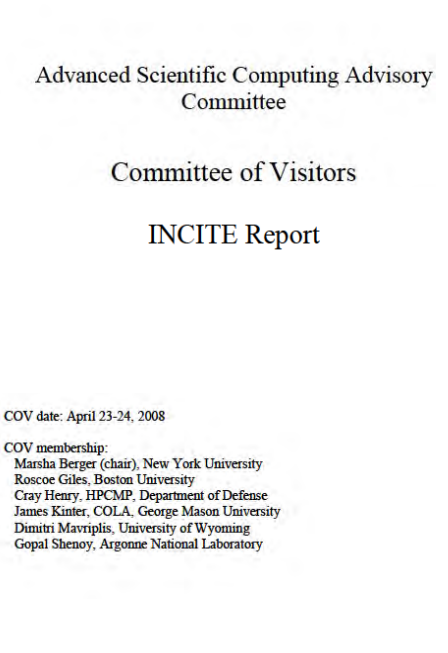
- Reviewers: Domain experts drawn from institutions worldwide

Criteria for new proposals	Criteria for renewals*
• Scientific and/or technical merit • Appropriateness of proposal method • Team qualifications • Reasonableness of requested resources	• Change in scope • Met technical/scientific milestones • On track to meet future milestones • Impact relative to other proposals under consideration

*Assessment of renewals, as recommended by 2008 Committee of Visitors

2010 INCITE process improvements

- Introduced a feedback step for computational review
- Enhanced program transparency by providing reviewer comments to authors
  - Response to 2008 Committee of Visitors recommendation
- Created a “blue ribbon” peer review panel
- Initiated review of renewals
  - Response to 2008 Committee of Visitors recommendation
- Engaged ALCF and OLCF management teams and INCITE manager in selection of proposals



Advanced Scientific Computing Advisory Committee

Committee of Visitors

INCITE Report

COV date: April 23-24, 2008

COV membership:
Marsha Berger (chair), New York University
Roscoe Giles, Boston University
Cray Henry, HPCMP, Department of Defense
James Kinter, COLA, George Mason University
Dimitri Mavriplis, University of Wyoming
Gopal Shenoy, Argonne National Laboratory

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2010 INCITE panel reviewer survey results

Survey statement	Rating
The INCITE proposals discussed in the panel represent some of the most cutting-edge computational work in the field	4.5
The proposals were comprehensive and of appropriate length given the award amount requested	3.9
The science panel was sufficiently diverse to assess the range of research topics being considered	4.2
Having access to the center's computational readiness (CR) reports was valuable for my assessment of the proposals	4.4
Please rate your overall satisfaction with the 2010 INCITE Science Panel review process (including expected communications from INCITE management, guidance received, coordination, etc.)	4.7

Scale: 1 = strongly disagree/very dissatisfied; 5 = strongly agree/very satisfied

2011 INCITE process plans

- Post the reviewer questions with the call for proposals to increase transparency of assessment process for proposal authors
  - Recommended by 2008 Committee of Visitors
- Build review panel earlier in the year
- Identify potential opportunities for making referrals from INCITE to ERCAP
- Reassess and potentially redesign web-based form for proposal submittal
  - Increase ease of use
  - Accommodate recent and projected program growth
- Build relationships with other centers whose users have science challenges that would benefit from the scale of the INCITE resources

Contacts

For details about the INCITE program:

http://hpc.science.doe.gov
INCITE@DOEleadershipcomputing.org

For details about the ALCC program:

http://www.er.doe.gov/ascr/Facilities/ALCC.html
ALCC@Science.doe.gov