U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Update on INCITE

Paul C. Messina, Director of Science, ALCF

and

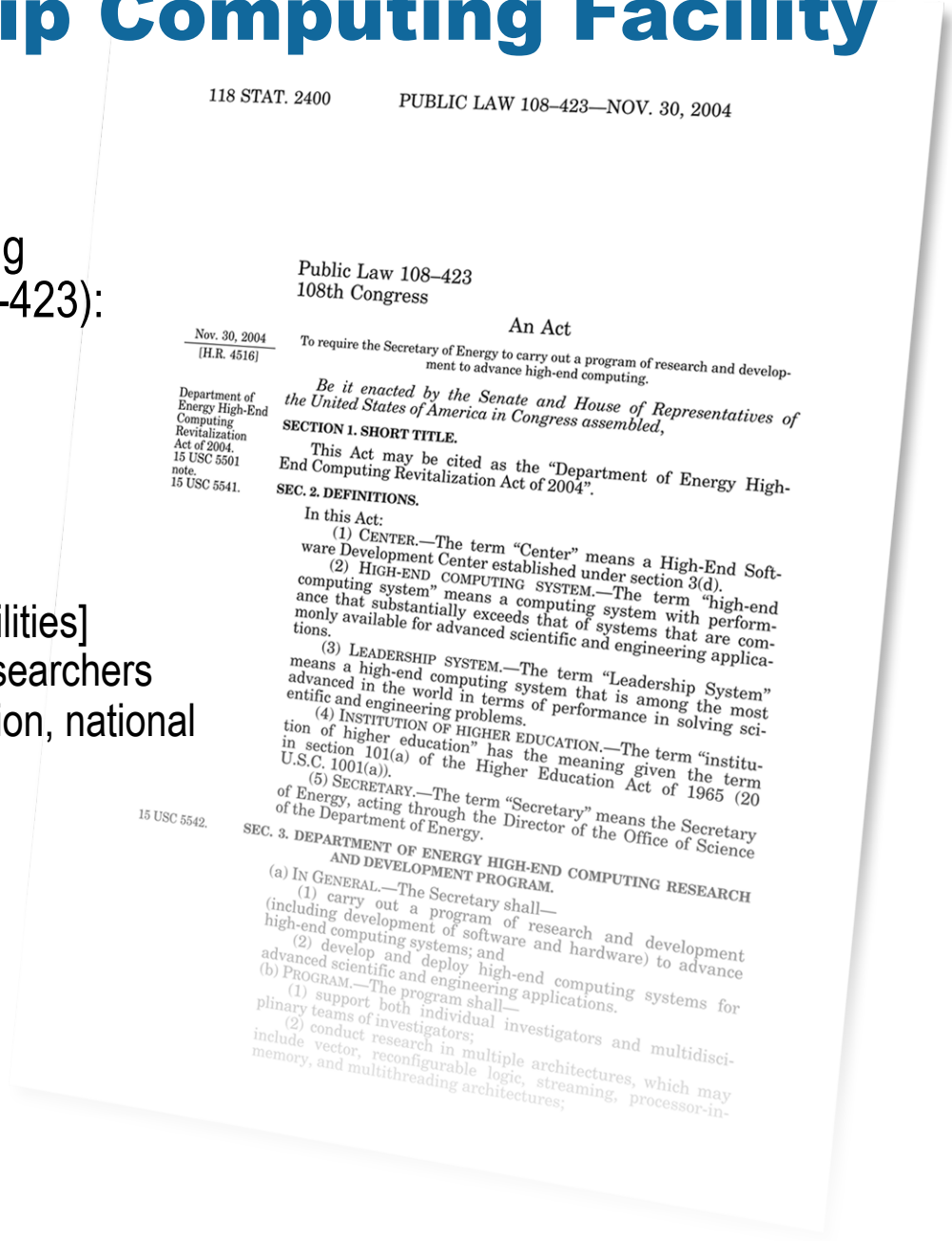
Julia C. White, INCITE Manager

whitejc@DOEleadershipcomputing.org

Origin of Leadership Computing Facility

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 in U.S. industry, institutions of higher education, national laboratories and other Federal agencies



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—

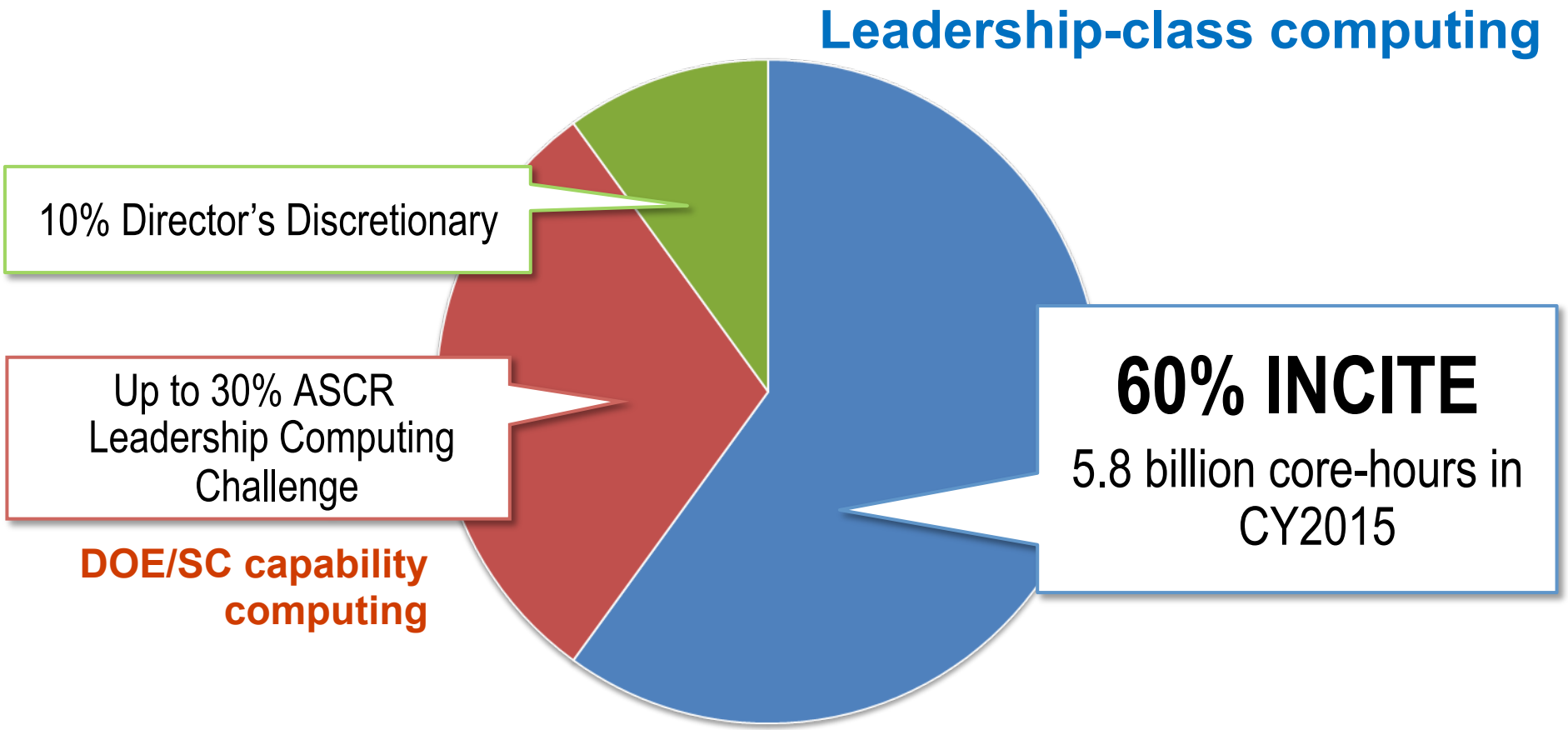
(1) support both individual investigators and multidisciplinary teams of investigators;

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

Titan and Mira

	INCITE Production Systems	
	Cray XK7 "Titan"	**IBM Blue Gene/Q "Mira"**
Node	16-Core AMD 6274 Opteron + NVIDIA K20x (Kepler)	16-Core PowerPC A2
Compute Nodes	18,688 hybrid nodes	49,152 nodes
Compute Node configuration	16 x86 cores + 14 GPU	16 PPC64 Cores
Aggregate Configuration	299,008 x86 Cores	786,432 PPC64 Cores
Memory/Node	32 GB x86 + 6 GB K20x	16 GB RAM per node
Memory/Core	2 GB x86	1 GB
Interconnect	Gemini	5D Torus
GPUs	18,688 K20x Keplers	None
Speed	27 PF	10 PF

Three primary ways for access to LCF
Distribution of allocable hours



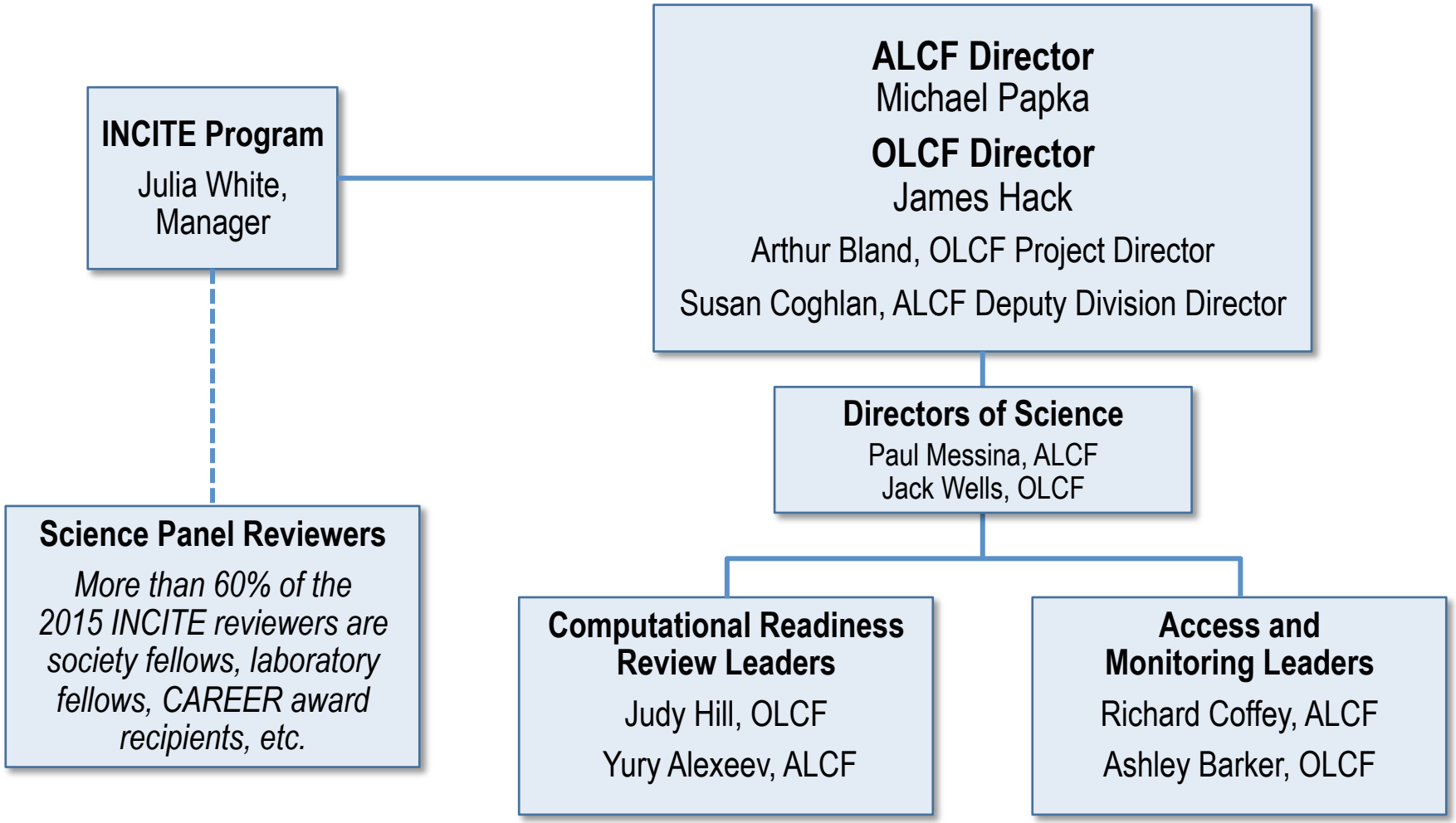
What is INCITE?

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

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 program organization



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 intensive runs that cannot be done anywhere else: *capability, architectural needs*

3 Eligibility criterion

- 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

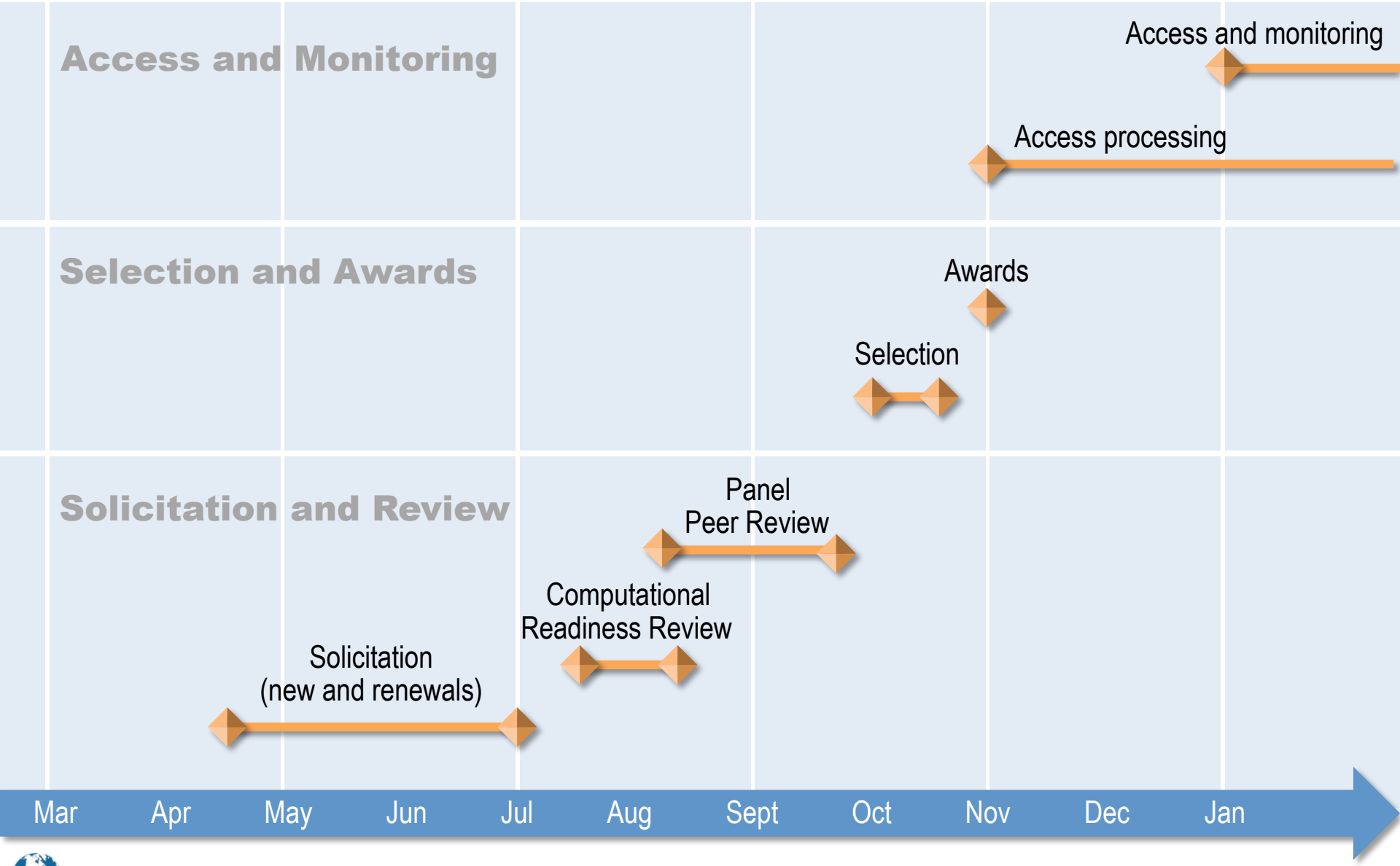
INCITE is open to researchers around the world in a broad array of domains

No designated number of hours for a particular science area

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

INCITE annual timeline



INCITE breakthroughs since inception

A few of the many science and engineering advances

Hours requested vs. allocated: *~2X per year* *~3X per year*

	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015
Hours allocated	4.9 M	6.5 M	18.2 M	95 M	268 M	889 M	1.6 B	1.7 B	1.7 B	4.7 B	5.8 B	5.8 B
Projects	3	3	15	45	55	66	69	57	60	61	59	56

Researchers solved the 2D Hubbard model and presented evidence that it predicts HTSC behavior ***Phys. Rev. Lett*** (2005)

Modeling of molecular basis of Parkinson's disease named #1 computational accomplishment ***Breakthroughs*** (2008)

Largest simulation of a galaxy's worth of dark matter, showed for the first time the fractal-like appearance of dark matter substructures. ***Nature*** (2008), ***Science*** (2009)

World's first continuous simulation of 21,000 years of Earth's climate history. ***Science*** (2009)

Largest-ever LES of a full-sized commercial combustion chamber used in an existing helicopter turbine **Compte Rendus de Mecanique** (2009)

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

Recovery from slow inactivation in potassium channels controlled by H_2O ***Nature*** (2013)

NIST proposes new standard reference materials from LCF concrete simulations

Calculation of the number of bound nuclei in nature, ***Nature*** (2012)

New method to rapidly determine protein structure, with limited experimental data ***Science*** (2010), ***Nature*** (2011)

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

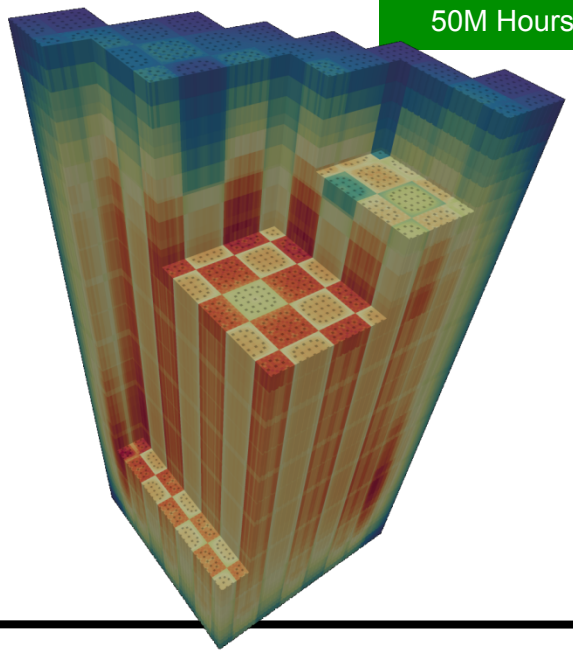
High-resolution reactor simulations predict startup conditions

John Turner
Oak Ridge National Laboratory
40M Hours, ES Project
50M Hours, INCITE 2013 Project

Science Objectives and Impact

Use Titan to predict the neutron fission power profile of the Westinghouse AP1000 reactor before startup using three approaches to solve the Boltzmann transport equation:

- Shift (Monte Carlo sampling)
- Denovo (discrete angular discretization)
- Insilico (improved diffusion approximation)



DENOVO is a component of the DOE CASL Hub, necessary to achieve CASL challenge problems.
Image Credit: John Turner

Application Performance

- Monte Carlo: 1 trillion particles (among the largest Monte Carlo calculations ever) > 230,000 Titan cores
- Denovo: Extremely fine-mesh calculations, GPU-accelerated speedup of 2x on overall application (4-6x on key computational kernel)
- Accelerated code is integrated into code base
- All 3 methods share identical input, which is a dramatic reduction in setup over traditional Monte Carlo codes
- GPU acceleration of Shift under way

Science Results

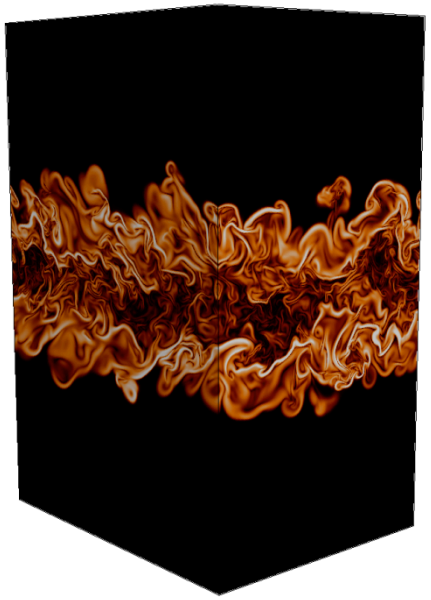
- Provide insight into core behavior of AP1000 before startup
- Strengthen confidence in predictions available using current industry tools
- Simulations predict reactor criticality, rod worth, and reactivity coefficients
- Three hours for each Shift simulation on Titan vs. one year for legacy Monte Carlo code
- Pioneering application successfully performed paves the way for what one day may become the standard approach to reactor simulations

The Complexities of Combustion

Jackie Chen
Sandia National Laboratories
79M Hours, OLCF Early Science Project
106M Hours, INCITE 2014 Project

Science Objectives and Impact

- Strategy: Use Titan to develop predictive models of turbulence in internal combustion engines and gas turbines.
- Objective: Employ S3D code to simulate a jet flame burning dimethyl ether and understand how a flame re-ignites.
- Impact: DNS and experimental data used to assess and develop predictive models for optimizing design of fuel efficient, clean vehicles and gas turbines using alternative fuels.



The logarithm of the scalar dissipation rate (that is, the local mixing rate) where white denotes high mixing rates and red lower mixing rates.

Performance Results

- ORNL's R. Sankaran and Cray's J. Levesque worked closely with team to optimize S3D on Titan.
- S3D was one of OLCF CAAR Early Science projects and the only one to use OpenACC.
- S3D runs 6x faster on Titan than on Jaguar due almost entirely to incorporation of OpenACC.
- From ExaCT codesign another 2X faster using Legion programming model and deferred execution runtime.

Science Results

- Simulated dimethyl ether for the first time – representative oxygenated biofuel with 32 species.
- S3D speedup on Titan enabled the team's largest ever Reynolds number at 13,050.
- Simultaneous imaging of formaldehyde and hydroxyl was evaluated to determine effectiveness at measuring peak heat release rate.
- Sim data verified method performed very well at predicting maximum release rate.
- Mechanism of re-ignition due to coupling of turbulence and finite-rate DME chemistry revealed.

A. Bhagatwala, *Proc. Combust. Inst.* (2014)

Direct Numerical Simulations of High Reynolds Number Turbulent Channel Flow

Robert D. Moser, University of Texas, Austin

ESP and INCITE 2013
175 M hours

Impact and Approach

- About 28% of U.S. energy resources are expended on transportation, in which the turbulence caused by the motion of fluid past walls governs much of the energy loss.
- Using a hybrid-spectral DNS code, this simulation on 524,288 cores of Mira aimed at a more complete understanding of wall-bounded turbulence.
- DNS at $Re_\tau = 5200$ is the highest Reynolds number ever simulated to explore the physics in the overlap region between near-wall and out-layer turbulence; key to understanding high Re turbulent wall layers.
- Myoungkyu Lee and Nicholas Malaya and Robert D. Moser, *"Petascale Direct Numerical Simulation of Turbulent Channel Flow on up to 786K Cores"* Proc. SC13

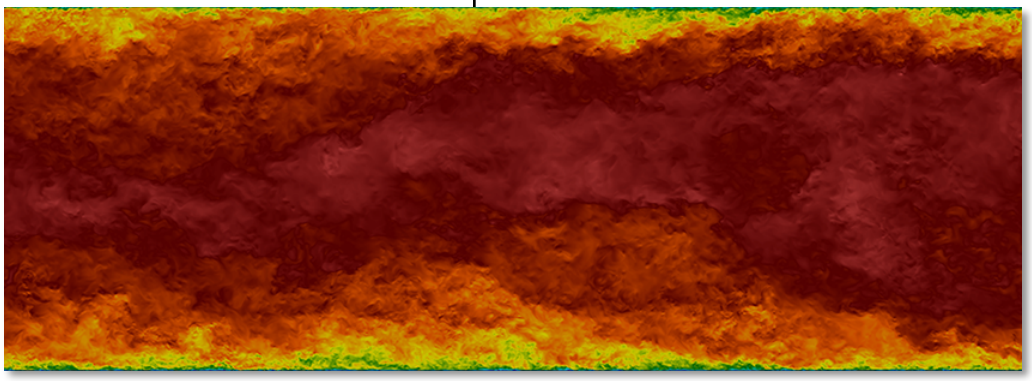
Accomplishments

- Highly resolved turbulent field reveals that large scale motions contribute significantly to the turbulent intensity and Reynolds shear stress.
- Results are being used as a standard for development and validation of turbulence models (140 TB). Results are available at: turbulence.ices.utexas.edu

ALCF Contributions

- Collaboration with Ramesh Balakrishnan and Jeff Hammond led to improved management of cache & execution threads resulting in 2x performance increase.
- Minimizing inter-memory access between OpenMP threads, led to near-perfect OpenMP scalability.

Depiction of the instantaneous streamwise velocity component over a section of the simulated channel.



Hydrogen-on-Demand Using Lithium Aluminum Particles

Priya Vashishta, University of Southern California

INCITE 2013
200M hours

Impact and Approach

- On-demand hydrogen production for hydrogen-powered vehicles.
- Investigated chemical reaction for best generation of hydrogen
- Understand atomistic mechanisms from experiment: X. Chen et al., *Int. J. Energy Res.* 2013; **37**:1624-1634
- K. Shimamura, F. Shimojo, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta, Nano Lett., 2014, 14(7), pp. 4090-4096
- Quantum molecular dynamics (QMD) simulations on Blue Gene/Q used roughly half of Mira resource for several days.
- *Dr. James Davenport, Program Manager of Theoretical Condensed Matter Physics , Division of Materials Science and Engineering, BES (Grant Number DE-FG02-04ER46130) supported this research.*

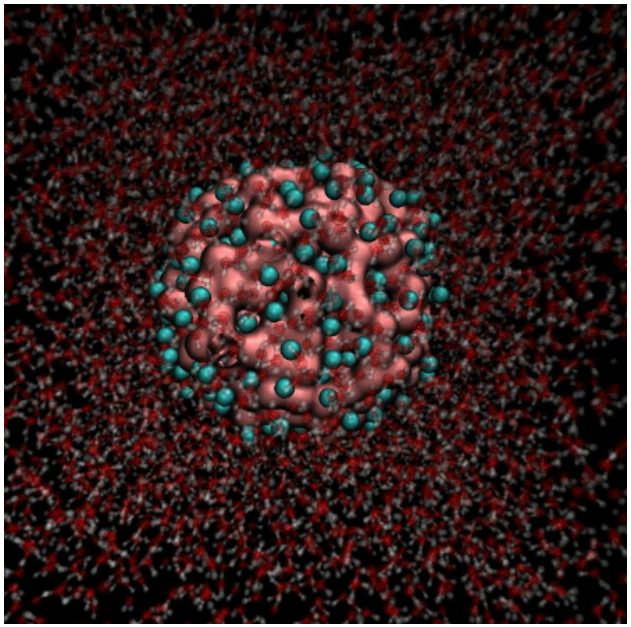
Accomplishments

- Demonstrated orders-of-magnitude acceleration of the reaction rate and higher yield by alloying Al nanoparticles with Li. Reaction rates and yield are high enough for industrial use.
- Revealed key nanostructural features for on-demand production of hydrogen gas from water using LiAl alloy nanoparticles. Production rate independent of nanoparticle size.

(Right) LiAl particle in water. White, red and cyan spheres are H, O and Li atoms, respectively, whereas the valence charge density colored in magenta is centered at Al atoms . 16,611 atoms are present in the simulation cell.

ALCF Contributions

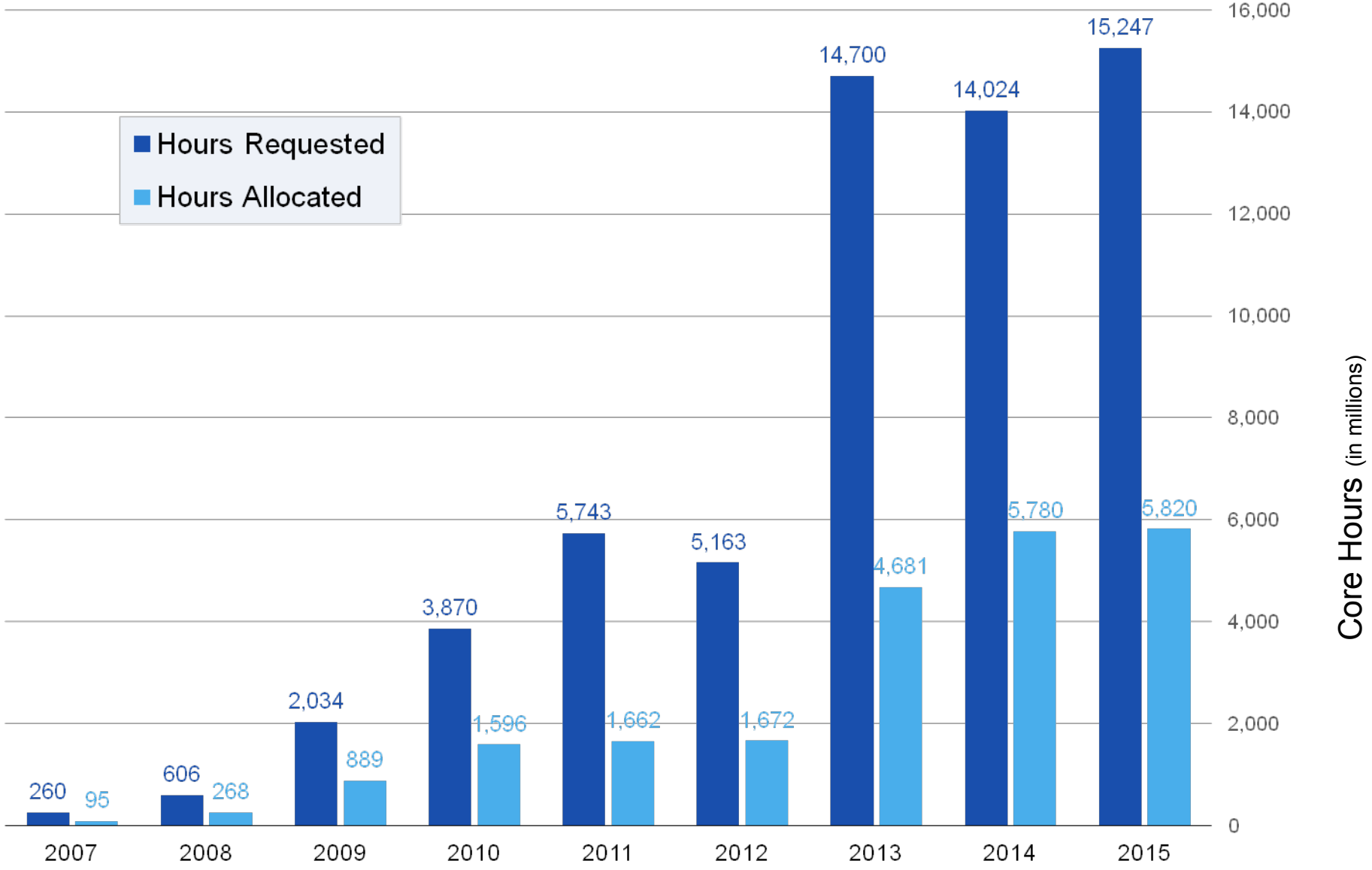
- Based on work started at Mira Performance Boot Camp, FLOP rate was doubled by their team with the help of Nichols Romero (ALCF) and Robert Walkup (IBM).
- Production runs used 50% - 100% of Mira (97% of use on > 1/3 of Mira)



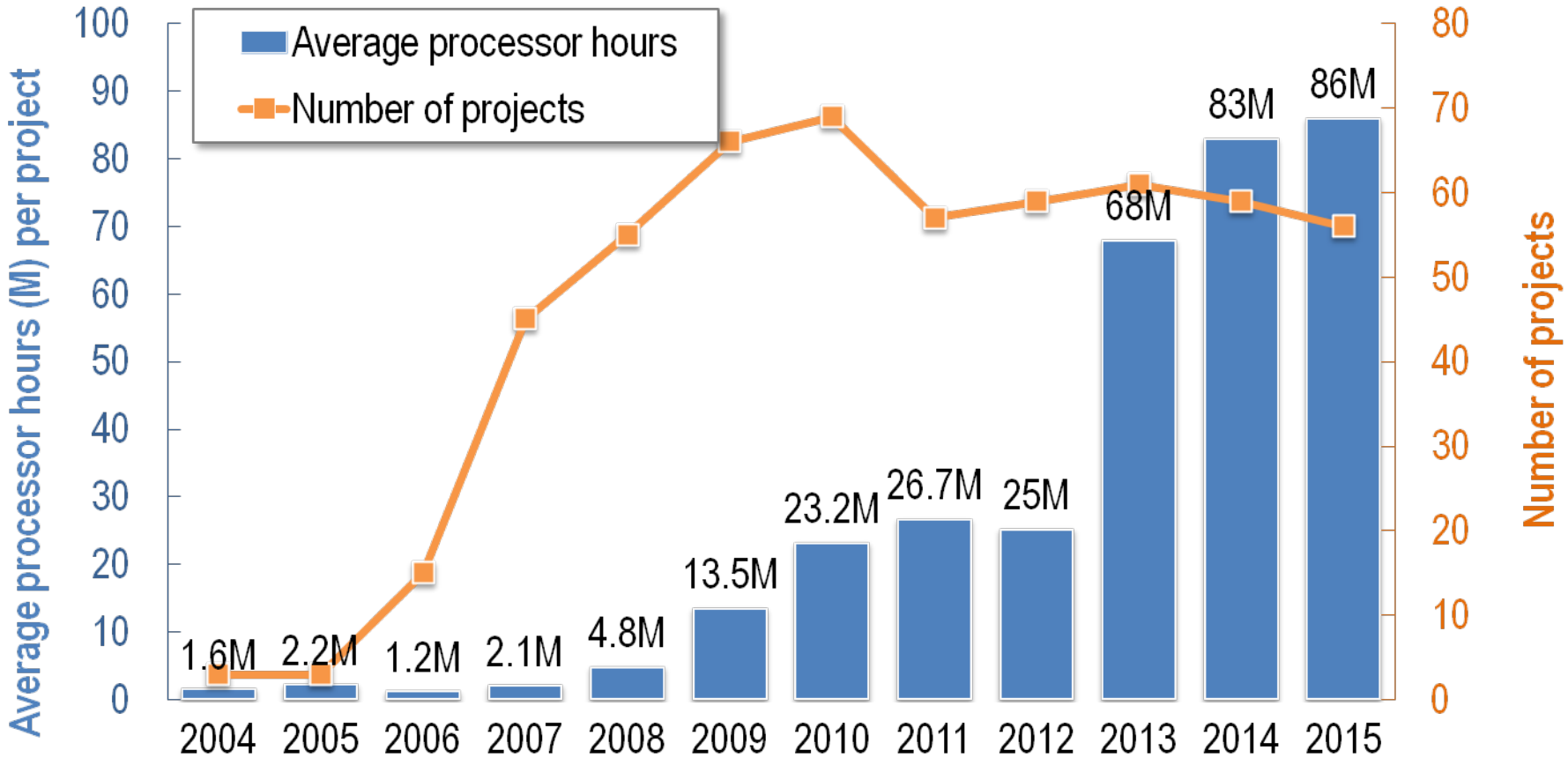
- *Computing resources for this DOE supported research were provided by the INCITE program.*

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

Demand versus available INCITE hours



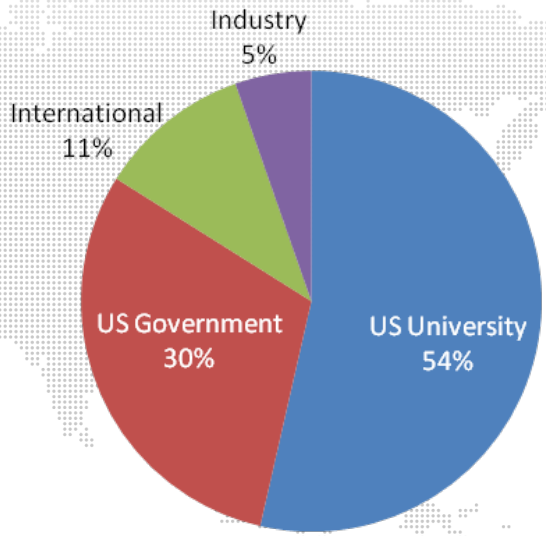
Size of INCITE awards



2015 INCITE award statistics

- Request for Information helped attract new projects
- Call closed June 27th, 2014
- Total requests **~15 billion core-hours**, an increase of 1 billion core-hours over last year's requests
- Awards of 5.8 billion core-hours for CY 2015
- **56 projects awarded of which 30 are renewals**

PIs by Affiliation (Awards)



Acceptance rates

27% of nonrenewal submittals and 91% of renewals

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

New proposals,* new PI's

*excluding renewal submittals

- **48%** of the PI's had never before led an INCITE proposal
  - 96 new proposals, 46 led by new PI's
- **23%** of non-renewal projects awarded time led by new PI's
  - 26 new projects awarded, 6 led by new PI's

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

2015 award statistics, by system

	Titan	Mira
Number of projects*	30	37
Average Project	75M	96.5M
Median Project	60M	89M
Total Awards (core-hrs in CY2015)	2.25B	3.57B

* Total of 56 INCITE projects (many of the projects received time on both Mira and Titan)

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Ab initio simulations of carrier transports in organic and inorganic nanosystems (Renewal)	Wang, Lin-Wang (LBNL)	25,000,000	
Accelerated Climate Modeling for Energy	Taylor, Mark (SNL)	50,000,000	140,000,000
Accelerator Modeling for Discovery	Amundson, James (Fermilab)		60,000,000
Adaptive Detached Eddy Simulation of a High Lift Wing with Active Flow Control	Jansen, Kenneth (University of Colorado)		70,000,000
Advancing Models for Multiphase Flow and Transport in Porous Medium System (Renewal)	McClure, James (Virginia Tech)	60,000,000	
Approaching Exascale Models of Astrophysical Explosions	Zingale, Michael (Stony Brook University)	50,000,000	

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Catalyst Support Interactions	Abild-Pedersen, Frank (Stanford University/SLAC)		50,000,000
CESM Century-Scale Climate Experiments with a High-Resolution Atmosphere (Renewal)	Washington, Warren (UCAR)		200,000,000
Characterizing Large-Scale Structural Transitions in Membrane Transporters	Tajkhorshid, Emad (University of Illinois)	96,000,000	
Computational Actinide Chemistry: Reliable Predictions and New Concepts (Renewal)	Dixon, David (University of Alabama)	150,000,000	
Computational spectroscopy of heterogeneous interfaces	Galli, Giulia (University of Chicago)		180,000,000
Cosmic Reionization On Computers	Gnedin, Nickolay (Fermilab)		74,000,000

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Cosmological Simulations for Large-Scale Sky Surveys (Renewal)	Habib, Salman (ANL)	80,000,000	80,000,000
Designing O2 tolerant hydrogenases (Renewal)	Pande, Vijay (Stanford University)	13,000,000	
Direct Numerical Simulations and Robust Predictions of Cloud Cavitation Collapse	Koumoutsakos, Petros (ETH Zürich, Switzerland)		88,000,000
DNS of Turbulent Combustion Towards Fuel-Flexible Gas Turbines and IC Engines (Renewal)	Chen, Jacqueline (SNL)	106,000,000	
DNS/LES of Complex Turbulent Flows	Mahesh, Krishnan (University of Minnesota)		100,000,000
Dynamic and Adaptive Parallel Programming for Exascale Research	Harrison, Robert (BNL/Stony Brook University)		15,000,000

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
First-principles simulations of high-speed combustion and detonation (Renewal)	Khokhlov, Alexei (University of Chicago)		150,000,000
Frontiers in planetary and stellar magnetism through high-performance computing	Aurnou, Jonathan (UCLA)		83,000,000
Global Adjoint Tomography	Tromp, Jeroen (Princeton University)	50,000,000	
High Frequency Ground Motion Simulation for Seismic Hazard Analysis	Jordan, Thomas (USC)	119,000,000	48,000,000
High-fidelity simulation of tokamak edge plasma transport (Renewal)	Chang, Choong-Seock (Princeton Plasma Physics Laboratory)	170,000,000	100,000,000
High-Fidelity Simulations of Gas Turbine Stages with GPU Acceleration	Michelassi, Vittorio (General Electric)	40,000,000	

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Innovative Simulations of High-Temperature Superconductors (Renewal)	Maier, Thomas (ORNL)	60,000,000	
Large Eddy Simulations of combustor liner flows (Renewal)	Dord, Anne (General Electric)		89,000,000
Large-Eddy Simulation of the Bachalo-Johnson flow, with shock-induced separation	Spalart, Philippe (Boeing)		135,000,000
Large-scale coupled-cluster calculations of supramolecular wires (Renewal)	Jørgensen, Poul (Aarhus University, Denmark)	48,000,000	
Lattice QCD (Renewal)	Mackenzie, Paul (Fermilab)	100,000,000	180,000,000
Linkages between Turbulence and Reconnection in Kinetic Plasmas (Renewal)	Daughton, William (LANL)	60,000,000	

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Multiscale Simulations of Human Pathologies (Renewal)	Karniadakis, George (Brown University)	25,000,000	45,000,000
Non-covalent bonding in complex molecular systems with quantum Monte Carlo (Renewal)	Alfe, Dario (University College London, UK)	80,000,000	68,000,000
Nuclear Structure and Nuclear Reactions (Renewal)	Vary, James (Iowa State University)	104,000,000	100,000,000
Nucleation and growth of colloidal crystals using highly scalable Monte Carlo	Glotzer, Sharon (University of Michigan)	55,000,000	
Parameter studies of Boussinesq flows (Renewal)	Kurien, Susan (LANL)		44,000,000
Particle acceleration in shocks: from astrophysics to laboratory in silico (Renewal)	Fiuza, Frederico (LLNL)		110,000,000

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Performance Evaluation and Analysis Consortium (PEAC) End Station (Renewal)	Oliker, Leonid (LBNL)	45,000,000	45,000,000
Petascale Simulation of Magnetorotational Core-Collapse Supernovae	Couch, Sean (University of Chicago)		50,000,000
Petascale Simulations of Laser Plasma Interaction Relevant to IFE	Tsung, Frank (UCLA)		90,000,000
Petascale Simulations of Self-Healing Nanomaterials (Renewal)	Kalia, Rajiv (USC)		180,000,000
Predictive and insightful calculations of energy materials (Renewal)	Kent, Paul (ORNL)	50,000,000	
Predictive Materials Modeling for Li-Air Battery Systems (Renewal)	Curtiss, Larry (ANL)		50,000,000

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
QMC Simulations DataBase for predictive modeling and theory (Renewal)	Ceperley, David (University of Illinois)	85,000,000	100,000,000
Quantum Monte Carlo Simulations of Hydrogen and Water Ice (Renewal)	Needs, Richard (University of Cambridge, UK)	80,000,000	
Quark flavors and conserved charges at finite density in the QCD phase diagram	Bellwied, Rene (University of Houston)		150,000,000
Reactive MD simulations of electrochemical oxide interfaces at mesoscale (Renewal)	Sankaranarayanan, Subramanian (ANL)		40,000,000
Scalable first principles calculations for materials at finite temperature (Renewal)	Eisenbach, Markus (ORNL)	150,000,000	

2015 INCITE awards (core-hrs)

Project Title	PI	Titan	Mira
Scalable System Software for Parallel Programming (Renewal)	Latham, Robert (ANL)		25,000,000
Shutdown and recovery of the barrier function of human skin	Klein, Michael (Temple University)	92,000,000	
Simulation of correlated electrons for superconducting materials	Wagner, Lucas (University of Illinois)		106,000,000
Simulation of fundamental energy conversion processes in the cell	Schulten, Klaus (University of Illinois)	150,000,000	
SiO2 Fracture: Chemomechanics with a Machine Learning Hybrid QM/MM Scheme (Renewal)	Kermode, James (King's College London, UK)		125,000,000
State-of-the Art Simulations of Liquid Phenomena	Gordon, Mark (Iowa State University)		200,000,000

2015 INCITE awards (core-hrs)

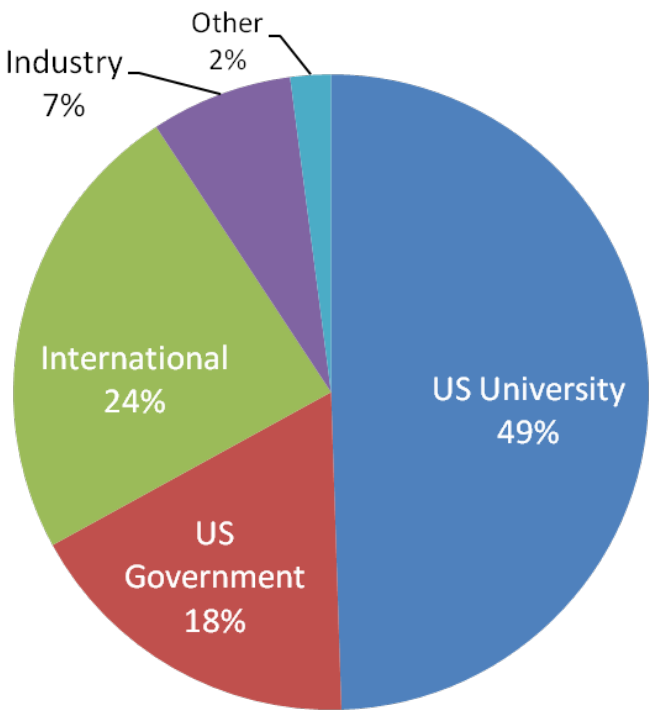
Project Title	PI	Titan	Mira
Studies of large conformational changes in biomolecular machines (Renewal)	Roux, Benoit (University of Chicago)		120,000,000
Targeting Cancer with High Power Lasers	Bussmann, Michael (Helmholtz-Zentrum Dresden-Rossendorf, Germany)	57,000,000	
Towards Breakthroughs in Protein Structure Calculation and Design	Baker, David (University of Washington)		80,000,000

2015 INCITE Panels

97 science experts participated in the 2015 INCITE panel review.

- 60+% of the reviewers include:
  Society Fellows (AAAS, APS, IEEE, etc),
  NSF or DOE Early CAREER,
  Laboratory Fellows,
  National Academy members,
  Department Chairs

- 48% participated in the
  2014 INCITE review



Reviewer Affiliation

2015 INCITE Panel questionnaire

*Scores range from 1 to 5 where 1 is "strongly disagree" and 5 is "strongly agree."

Questionnaire*	2015
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.	4.2
The science panel was sufficiently diverse to assess the range of research topics being considered.	4.5
Please rate your overall satisfaction with the 2015 INCITE Science Panel review process. (ranging from 1-"very dissatisfied" to 5-"very satisfied)	4.8

Contacts

For details about the INCITE program:

http://www.doeleadershipcomputing.org
INCITE@DOEleadershipcomputing.org

Fact sheets for 2015 awards are online

http://www.doeleadership computing.org/awards/2015INCITEFactSheets.pdf

Thank you