U.S. DEPARTMENT OF ENERGY

INCITE

LEADERSHIP COMPUTING

INCITE Overview

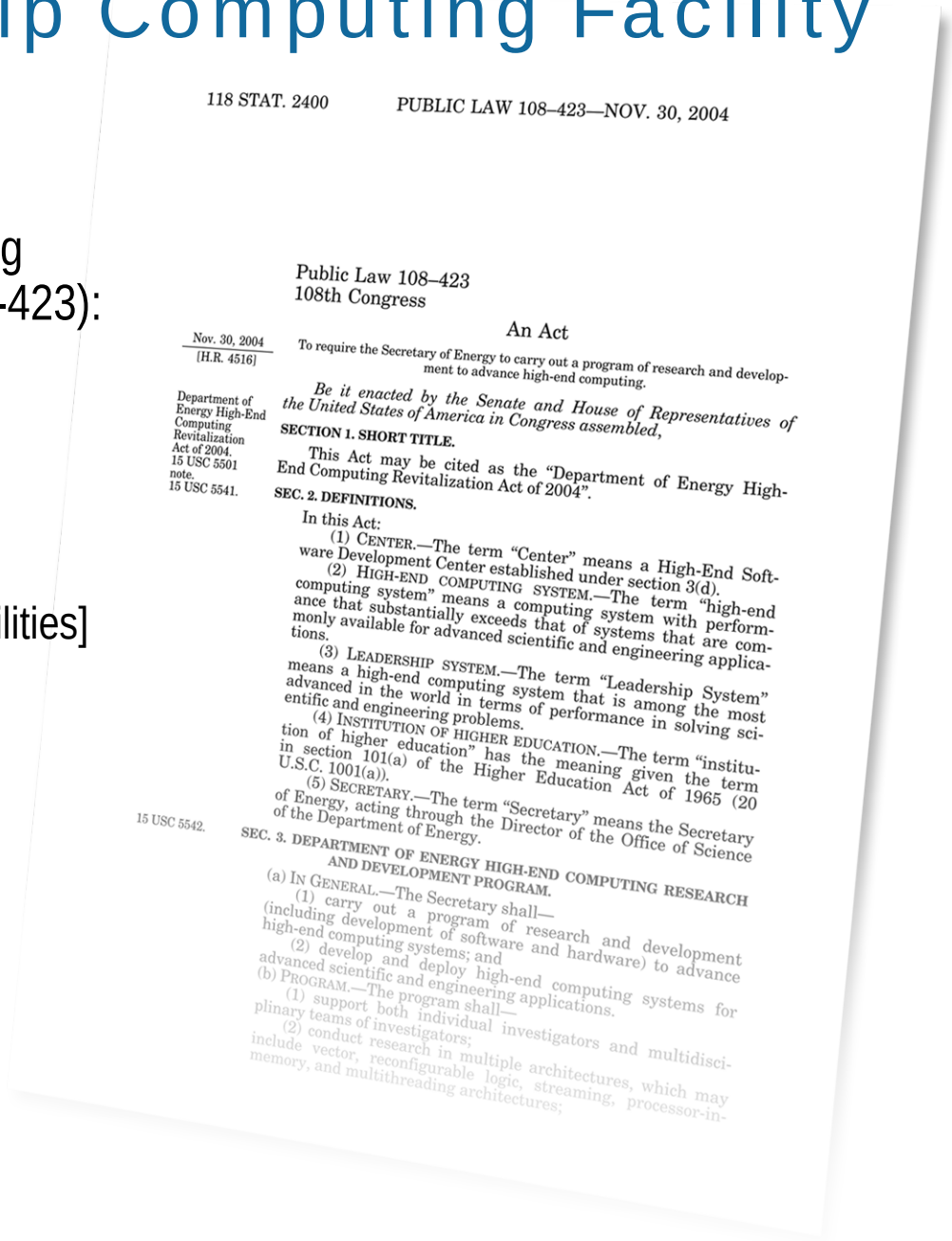
Lattice QCD Computational Science Workshop
April 30, 2013

Julia C. White, INCITE Manager

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

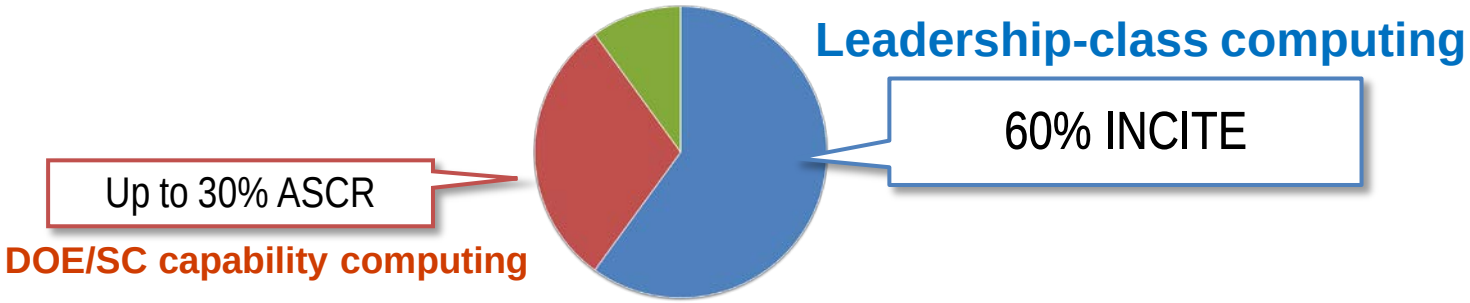
(2) develop and deploy high-end computing systems for advanced scientific and engineering applications.

(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;

Separation of selection processes for leadership-class computing and DOE capability computing



Total LCF allocable resource time

2008 ASCAC Committee of Visitors Recommendation 1

"The selection processes for leadership class and DOE capability class computing should be separated. A significant portion … of computational resources should be allocated to high-end DOE capability-class computing using a similar INCITE-type process."

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 breakthroughs since inception

A few of the many science and engineering advances

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

Hours allocated	4.9M	6.5M	18.2M	95M	268M	889M	1.6B	1.7B	1.7B	*5B*
Projects	3	3	15	45	55	66	69	57	60	61

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

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

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**

NIST proposes new standard reference materials from LCF concrete simulations

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

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*

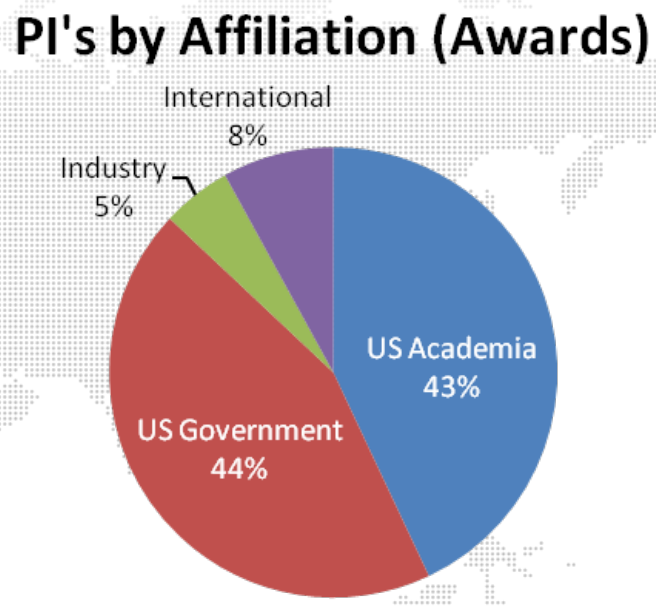
3 **Eligibility criterion**

- 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

2013 INCITE statistics

- Request for Information helped attract new projects
- Call closed June 27th, 2012
- Total requests ~15 billion core-hours, 3x more than the 5 billion core-hours requested last year
- Number of proposals submitted increased nearly 20%
- Awards of ~5 billion core-hours for CY 2013
- 61 projects awarded of which 20 are renewals



Acceptance rates

33% of nonrenewal submittals and 100% of renewals

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

2013 award statistics, by system

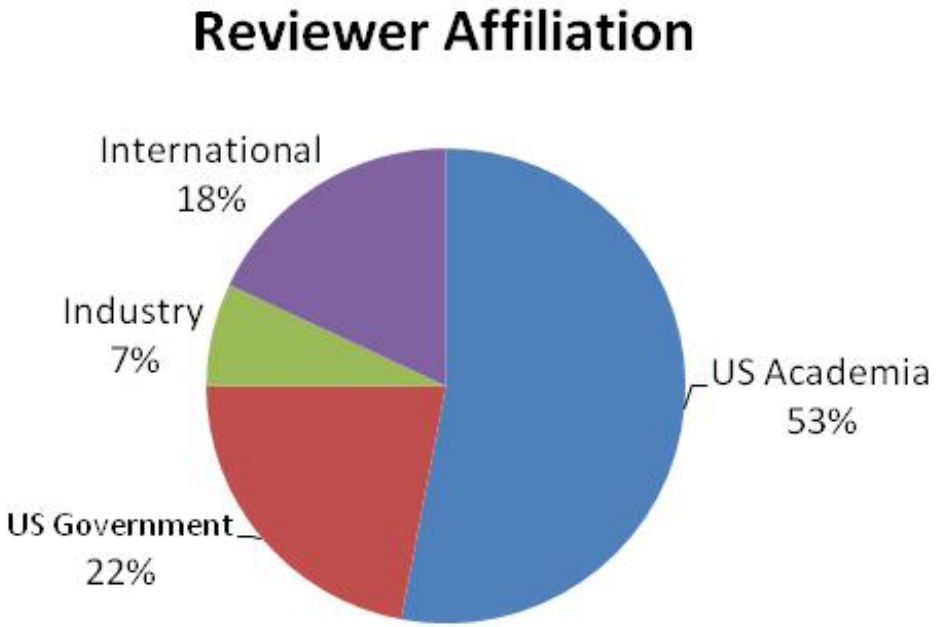
	Jaguar	Titan	Mira	Intrepid	
	2012 INCITE	2013 INCITE	2013 INCITE	2012 INCITE	2013 INCITE
Number projects*	35	32	27	31	27
Average Project	27M	58M	78M	24M	27M
Median Project	23M	49.5M	45M	20M	25M

* Totals of 32 projects at the OLCF, 37 projects at the ALCF (many of the ALCF projects received time on both Mira and Intrepid)

	Titan	Mira	Intrepid
Total Awards (Hrs in CY2013)	1.84B	2.11B	0.721B

2013 INCITE panel peer reviewers

- > 50% (e.g. more than 40) of the reviewers are:
  - — Society fellows (AAAS, APS, SIAM, IEEE, etc),
  - — Agency awardees (ex. NSF Early Career),
  - — Laboratory fellows,
  - — National Academy members,
  - — National Society presidents
- 41% participated in the 2012 INCITE review

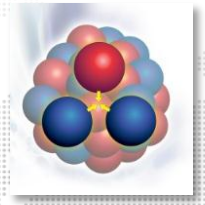
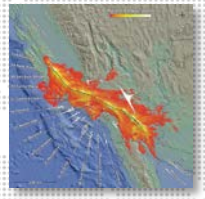


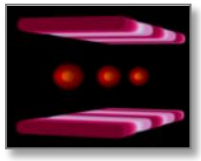
83 science experts participated in the 2013 INCITE panel review.

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 billion core-hours to be awarded for 2014 on the 27-petaflops Cray XK7 “Titan” and the 10-petaflops IBM BG/Q “Mira”
- Average award: 50+ million core-hours
- Individual awards will be up to several hundred million core-hours
- INCITE is open to any science domain
- INCITE seeks computationally intensive, large-scale research campaigns

2014 INCITE 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 2014.

April 15 – June 28, 2013

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

Proposal form: Outline

1	Principal investigator and co-principal investigators
2	Project title (80 characters)
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 impact of the work, objectives, benchmarking (15 pages)
	(C) Personnel justification & management plan
	(D) Milestone table
	(E) Publications resulting from INCITE Awards (*new*)
	(F) Request for Information – Data Management Plan (*new*)
9	Application packages
10	Proprietary and sensitive information
11	Export control
12	Monitor information

Narrative: Impact of the work

- DO explain the broader impact of the work
  - INCITE fields requests from DOE and non-DOE sources, numerous science areas, etc.
- DO connect milestones | hours needed | science impact

140M Titan core-hours equivalent to $7 million:
Describe in the proposal the potential return on this type of investment.
Outline how the time is to be used. Break down the thrust areas by milestones.

Narrative: New for 2014 Call for Proposals

- Publications resulting from INCITE awards
  - To show impact of the INCITE program, we ask authors to list the publications from previous INCITE awards to this project team for work related to the proposal under consideration
  - Include only publications with INCITE acknowledgements

Facilities MUST show impact of their resources

Narrative: New for 2014 Call for Proposals

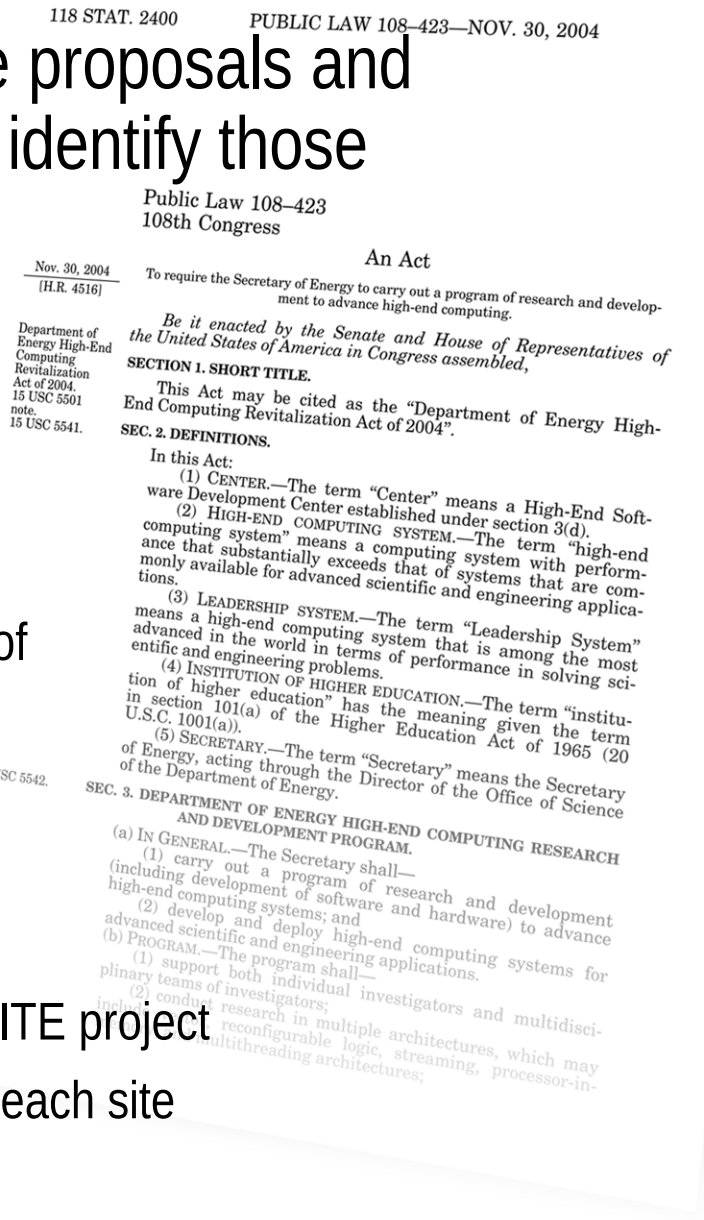
- Request for Information – Data Management Plan (DMP)
  - We plan to implement in future solicitations a requirement for a formal DMP as part of the proposal. Submit a short document, not to exceed one page, which describes your anticipated future data management strategies and needs. [Note: this is for INCITE management and will not be included in the materials sent to reviewers.]

This is part of the LCF 10-Year Strategic Plan

Awards decision-making

INCITE seeks grand-challenge-scale proposals and carries out a rigorous peer review to identify those of the highest potential impact.

- The INCITE Awards Committee identifies top-ranked proposals by:
  - peer-review panel rating and reports
  - additional considerations, e.g. promote use of HPC by underrepresented communities
- Individual awards granted are to:
  - Ensure sufficient allocation to enable all or part of the proposed scientific achievements
  - Maximize the scientific support for each INCITE project
  - Allocate all of the available INCITE hours at each site



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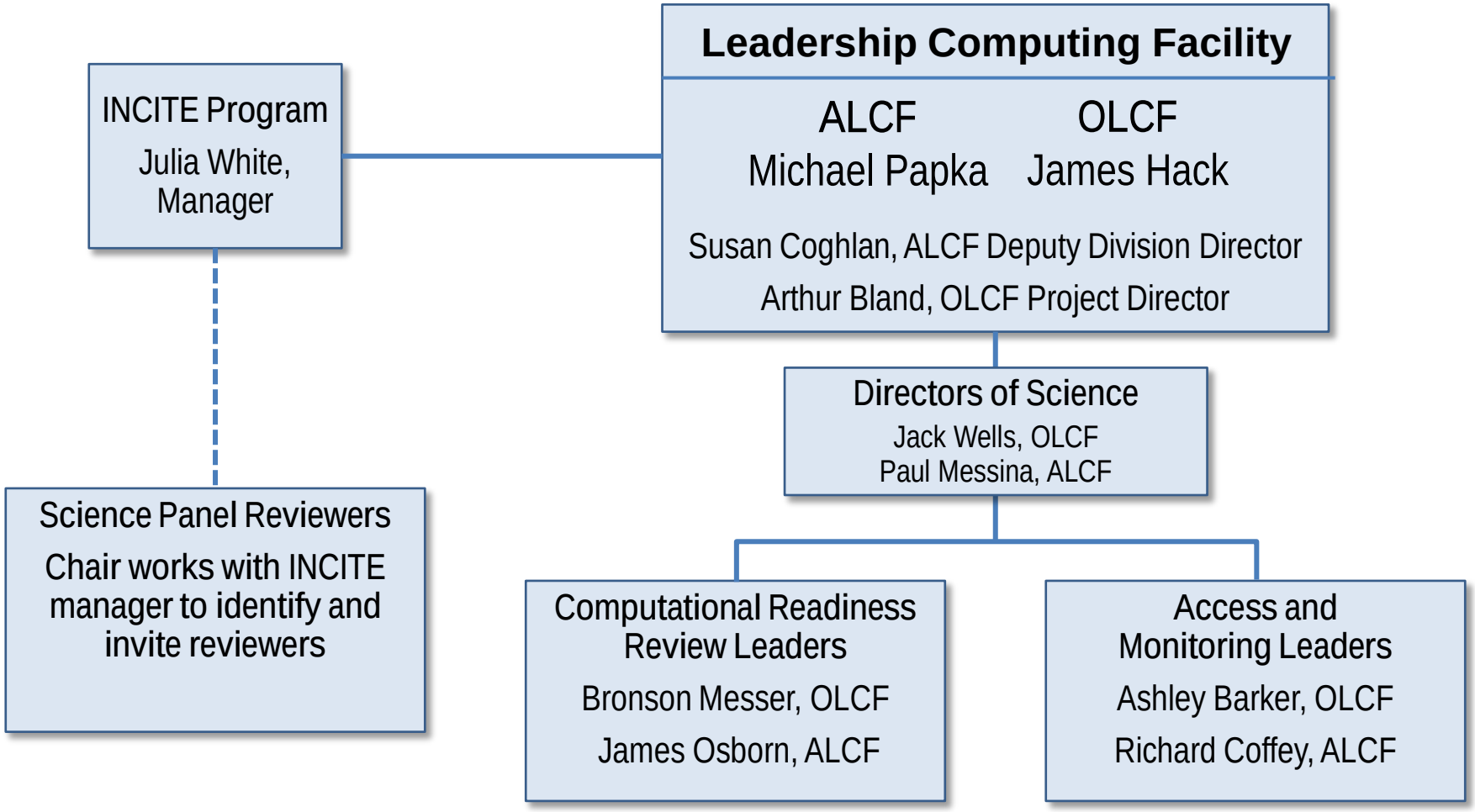
PI responsibilities

- Submit quarterly status updates (on supplied template)
  - Milestone reports
  - Publications, awards, journal covers, presentations, etc., related to the work
- Tell us about highlights on significant science/engineering accomplishments **as they occur**
- Complete annual surveys

Communications should be frequent:
Consider the value of the INCITE award. We expect to work closely with the project to generate highlights of research accomplishments.

INCITE program organization



Contacts

For details about the INCITE program:

www.doeleadershipcomputing.org – General information
proposals.doeleadershipcomputing.org – Proposal site
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