U.S. DEPARTMENT OF ENERGY | Office of Science

Overview of the ASCR Leadership Computing Challenge (ALCC)

ASCAC, March 31, 2014

Carolyn Lauzon
AAAS Science and Technology Policy Fellow at ASCR

ASCR Leadership Computing Challenge (ALCC) Basics

- **ASCR Leadership Computing Challenge (ALCC) is an allocation program for ASCR leadership and high-end computing resources**

- **ALCC originated in 2010**

- **ALCC mission:**

  Provide an allocation program for projects of interest to the Department of Energy (DOE) with an emphasis on high-risk, high-payoff simulations in areas directly related to the DOE mission and for broadening the community of researchers capable of using leadership computing resources.

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ALCC Allocates Time at ASCR Computing Facilities

Leadership Computing Facilities (LCFs)

Titan:
- Oak Ridge National Laboratory
- Peak performance of 27.1 Petaflops
- 18,688 Hybrid Compute Nodes

Mira:
- Argonne National Laboratory
- Peak performance of 10 Petaflops
- 49,152 Compute Nodes

National Energy Research Scientific Computing (NERSC) Research Scientific Computing<

Edison XC30:
- Lawrence Berkley National Laboratory
- Peak performance 2.4PF
- 124,608 processing cores

ALCC Complements Other Allocation Mechanisms (1/2)

- **Innovative and Novel Computing Theory and Experiment Program (INCITE)**
  - Supports open science , must use majority of machine
  - Allocations on LCFs

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  - DOE Office of Science allocation program
  - Allocations on NERSC

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  - DOE Office of Science allocation program
  - Allocations on NERSC
- **ASCR Leadership Computing Challenge (ALCC)**
  - Supports DOE mission science and broadening user community
  - Allocations on NERSC and LCFs

ALCC Complements Other Allocation Mechanisms (2/2)

	ERCAP	**ALCC**	INCITE
Science Mission	DOE-SC focus	**DOE focus**	• Open science • Must use majority of machine
% Machine Time / Site	80% NERSC	**30% LCF, 10% NERSC**	60% LCF
Management Location	SC offices	**ASCR**	LCFs
Duration of Award	One year	**One year**	Multi-year
Number of Awards (2013)	604	**39**	61
Project Size (mean, 2013)	1.9 M cpu-hours	**47 M cpu-hours**	70 M cpu-hours

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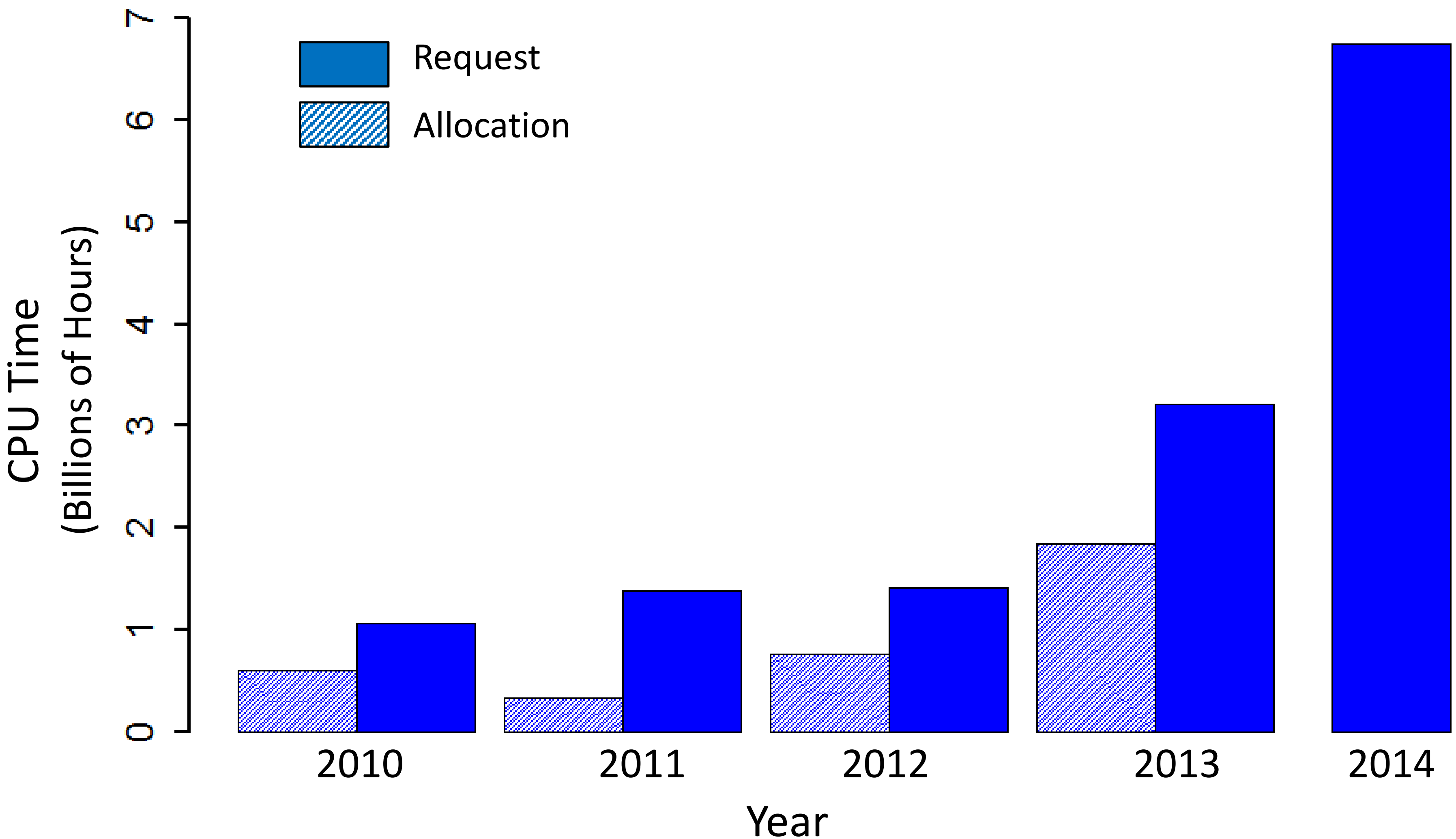
ALCC User Growth Since 2010

- **ALCC applicants are growing in number and are requesting more time.**
- **Growth reflects outreach efforts and the increasing ability of scientists and scientific codes to leverage HPC resources.**

Year	Applicant Count	Median Request (M cpu-hours)	Largest Request (M cpu-hours)
2010	29	20	223
2011	36	30	241
2012	35	30	316
2013	56	41	370
2014	77	62	800

ALCC Requested and Allocated Hours



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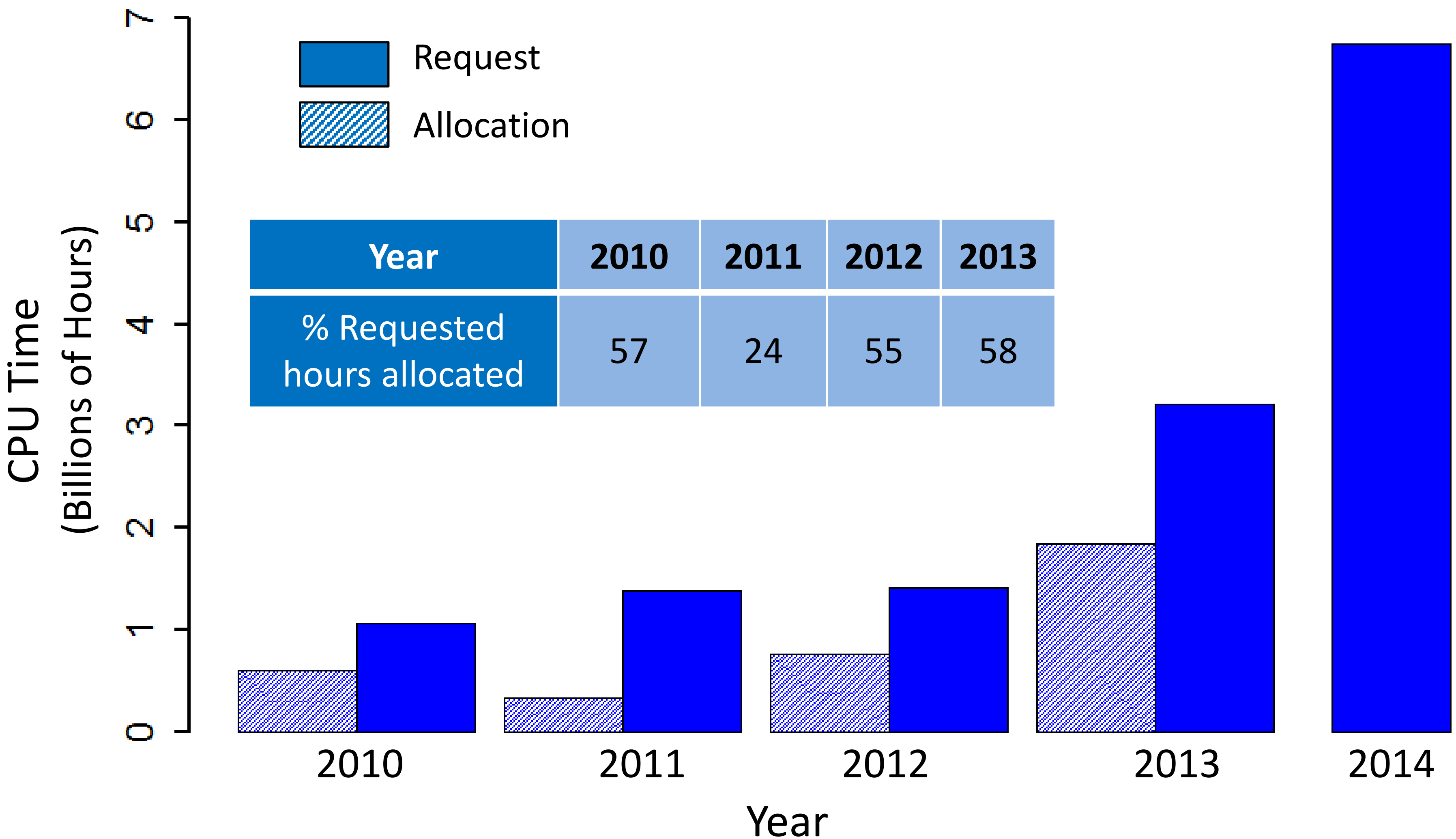

Year	2010	2011	2012	2013
% Requested hours allocated	57	24	55	58

What Are Science Drivers for Growth?

Methods for Deep Dive into Science Drivers (applies to slides 11-15)

- **Goal: Identify science drivers and scientific constituents that drive ALCC growth**

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- **Method: Bin proposals by topic area and investigate growth since 2010**
  - To best connect science drivers to DOE mission, ALCC proposals were binned according to alignment with DOE office missions:
    - Groupings:
      - 5 of the DOE Applied Offices (EERE, ARPA-e, Fossil Energy, Nuclear Energy, NNSA)
      - 6 DOE Basic Science Offices
      - Other (Weather, aeronautics, protein modeling for drug targets)

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  - Binning process:
    - (1) Proposals were assigned 1 binning only and crosscutting proposals were assigned to single best match.
    - (2) If a proposal identified DOE funding source, the funding was used to bin the proposal
    - (3) In all other cases, PI affiliation, institution, and proposal topic area were used to bin the proposal

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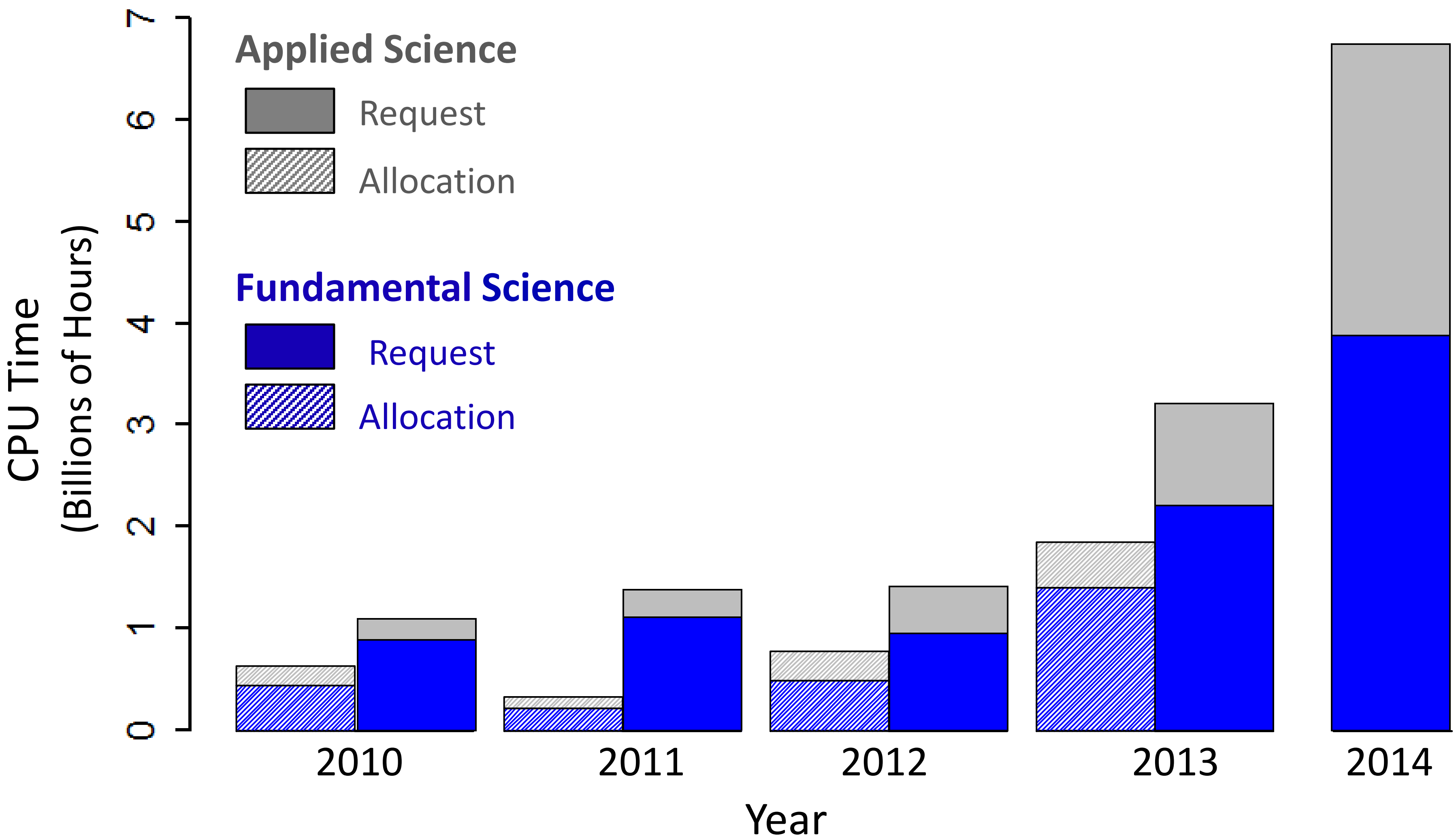
- **Note: Proposals binned into a DOE office were not necessarily funded by the office, but were considered to categorically fit the office mission. Data is subject to updates.**

Science Drivers for Growth: Fundamental Science and Applied Science



Science Drivers: Applied Science Topics

Other

- Turbomachinery
- Aeronautics
- Applied turbulence

ARPA-e

- Heat capture for Concentrated Solar Panels
- Protein Engineering

NE

- CASL
- NEAMS
- Reactor safety and efficiency

NNSA

- PSAAP
  - Laser plasma fusion
  - Turbulence

EERE

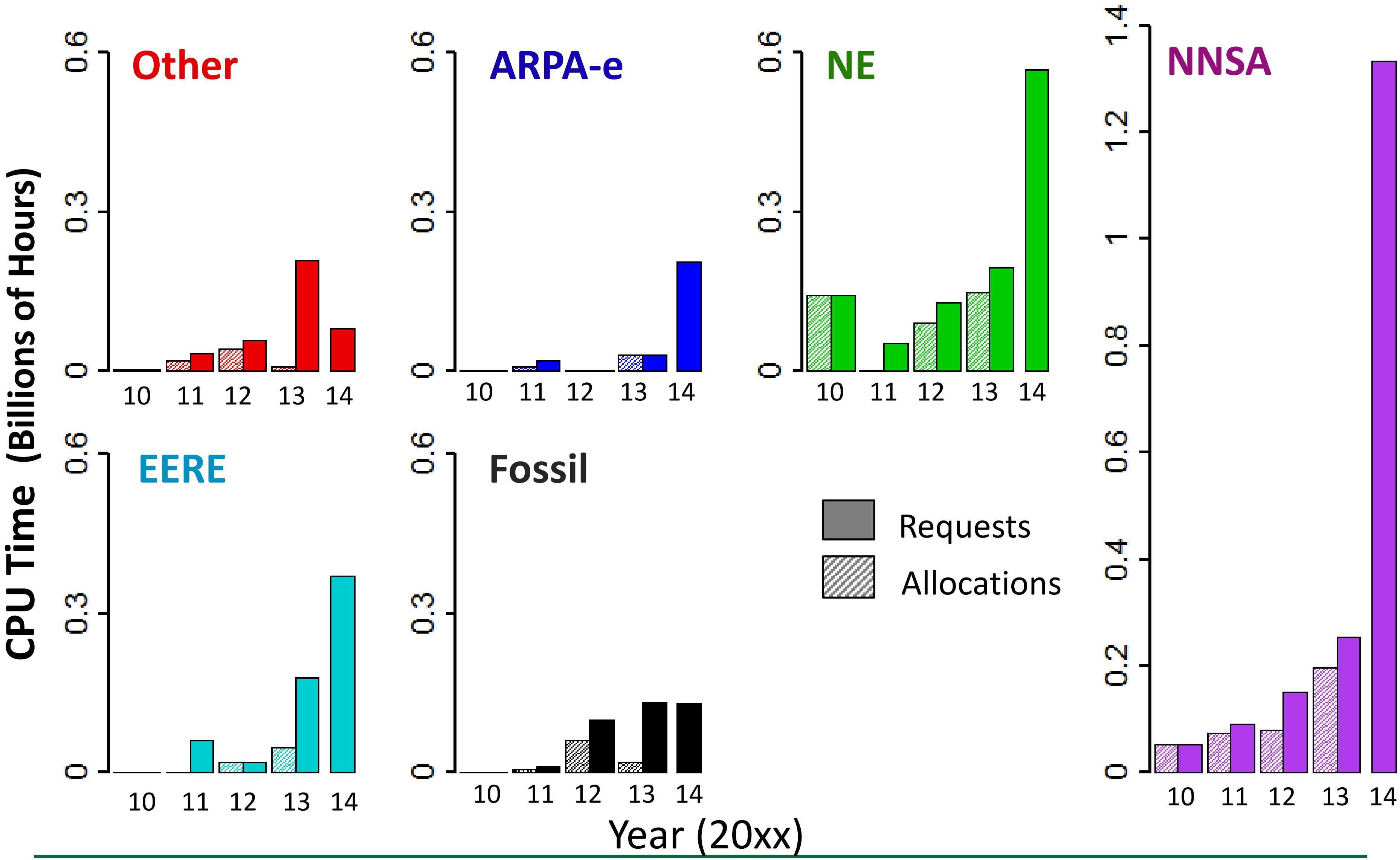
- Wind turbines
- Additive Manufacturing
- Hydropower
- Engine efficiency (turbulence, spray, combustion)

Fossil

- Carbon capture and sequestration

Acronyms: PSAAP- Predictive Science Academic Alliance Program, NEAMS – Nuclear Energy Advanced Modeling and Simulation, CASL- Consortium for Advanced Simulation of Light Water Reactors

Science Drivers: Growth in the Applied Sciences



Science Drivers: Basic Science Topics

ASCR

- SciDac
- ASCR Joule Metric
- Code development

HEP

- LHC modeling
- Cosmology

FES

- ITER simulations
- Laser plasma fusion

BES

- Materials science
- Chemistry
- Organic-Photovoltaics

BER

- Climate
- Subsurface modeling
- Biophysical modeling for bioenergy

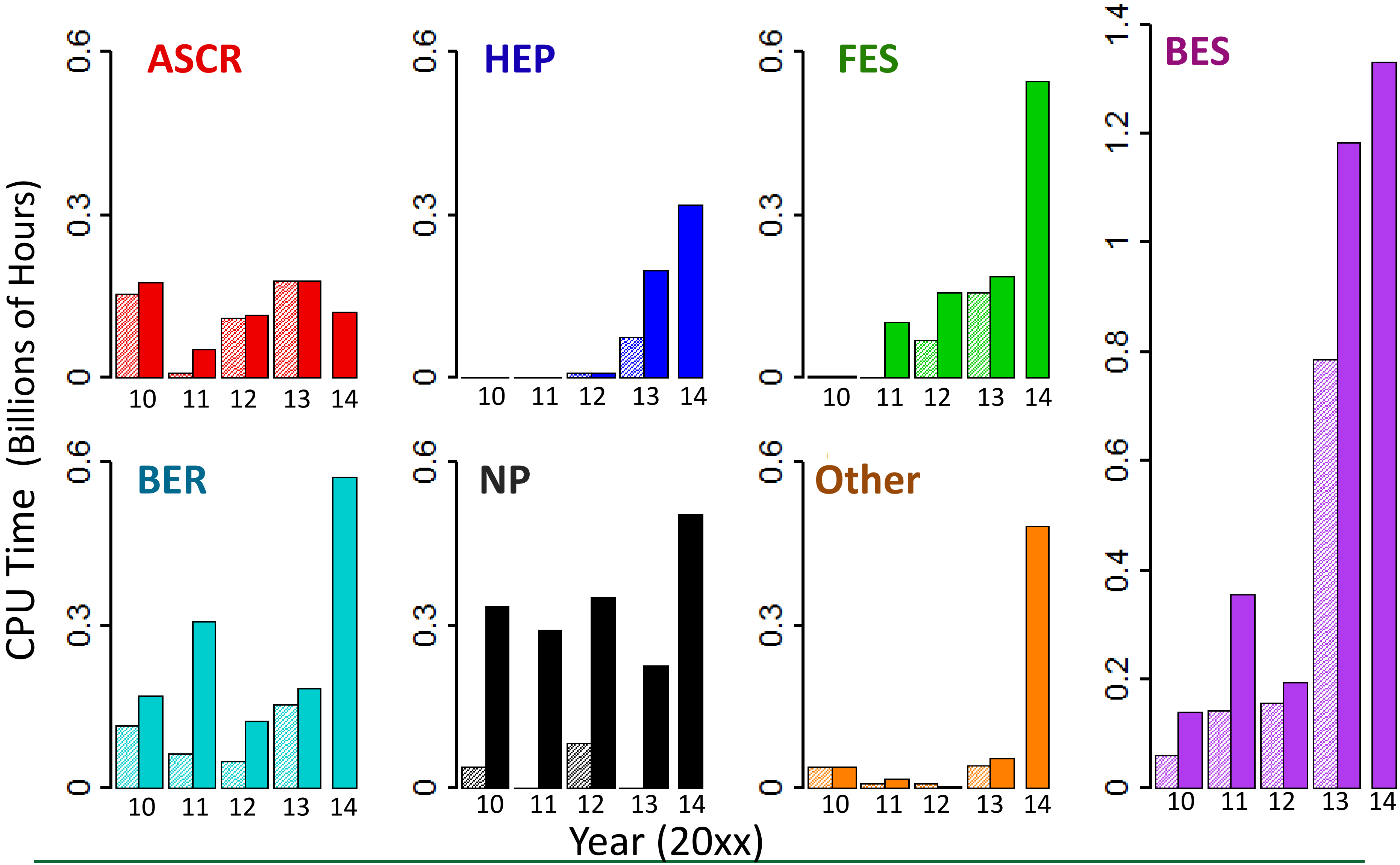
NP

- Quantum Chromodynamics
- Nuclear physics of supernovae
- Atomic physics

Other

- Basic science turbulence
- Earth science (NSF)
- Weather (NOAA)
- Protein modeling (NIH)
- Blood Flow (NIH)

Science Drivers: Growth in the Fundamental Sciences



ALCC Broadening Community of Users

- **77 PIs awarded time through ALCC**

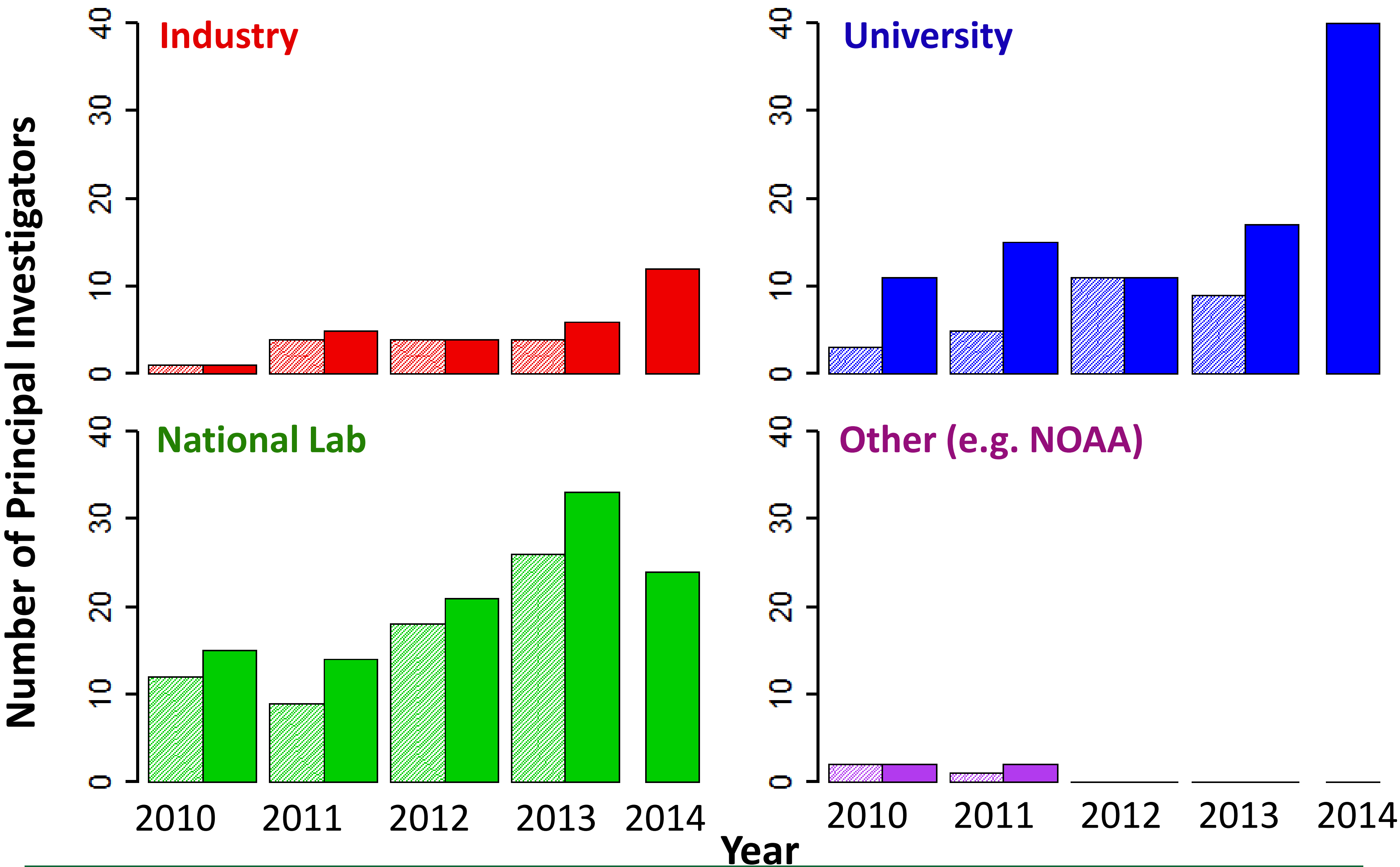
- **Number of New Users Awarded ALCC Time (New = new to INCITE or ALCC)**

Year	Number Awarded Proposals	Number New PIs	% New PIs
2010	18	14	78 %
2011	18	13	72 %
2012	31	18	58 %
2013	38	18	47 %

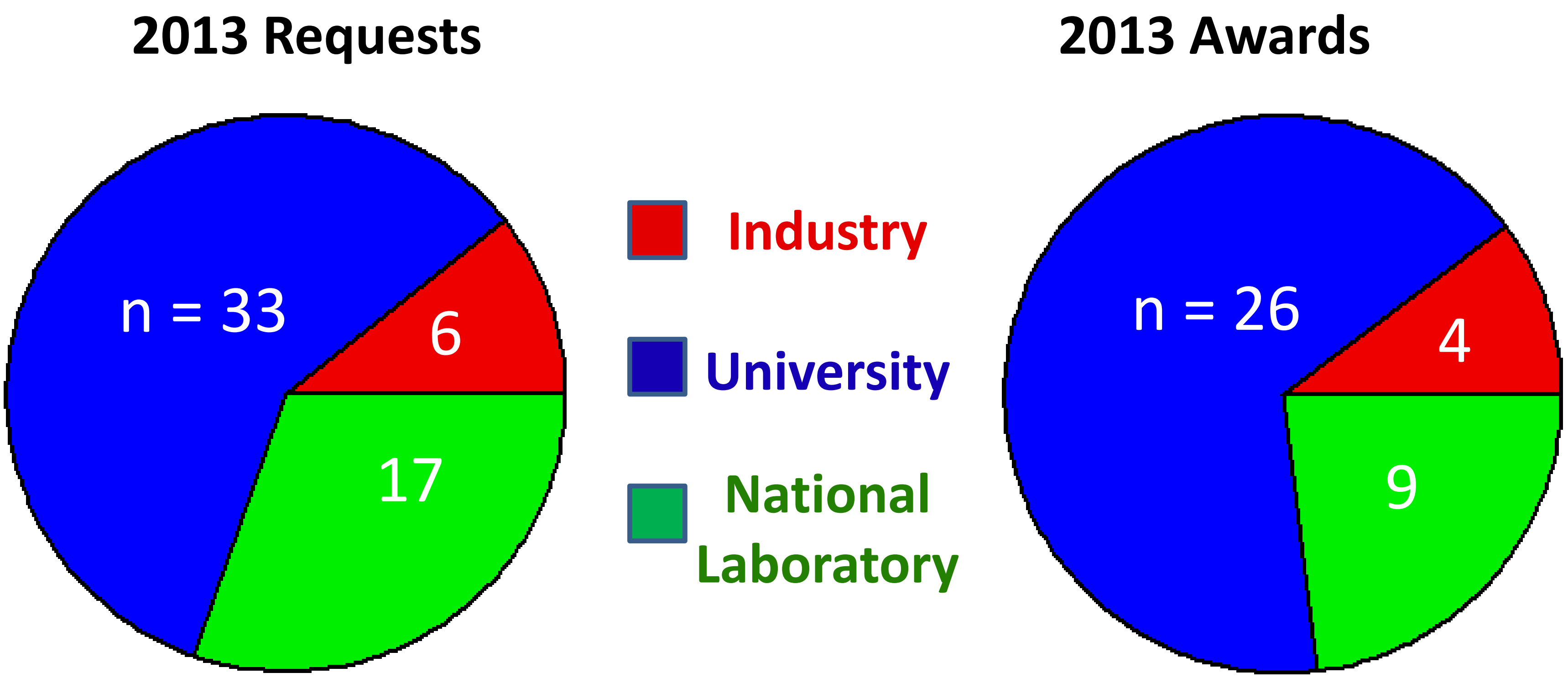
- **~13 % Of ALCC PIs later received INCITE awards**

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

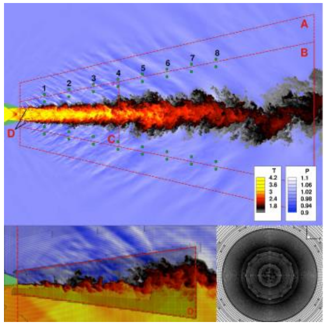
Community of Users: Principle Investigator Affiliations



2013 Number of Requests and Awards By Affiliation

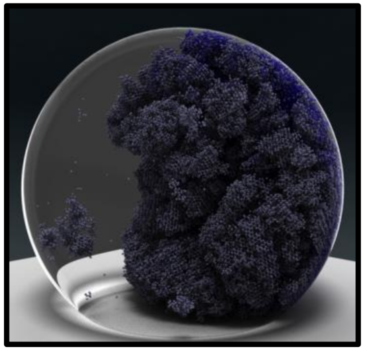


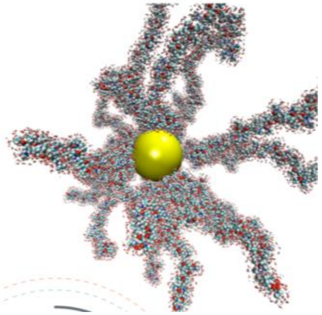
ALCC Supports High-impact DOE Mission Science



Turbulence Modeling, ALCF 150M
Parviz Moin *(Stanford U.).* Prediction of multiscale, multiphysics turbulent flow phenomenom. *Phys. Fluids* 2014 v26; *CSGF PhD Thesis*

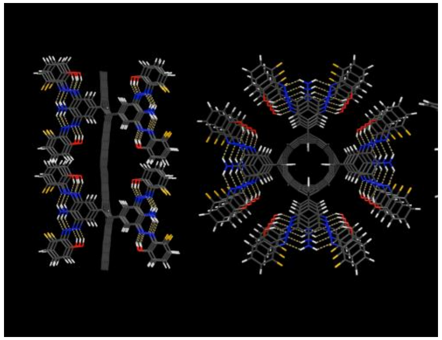
Nucleation of Ice, OLCF 40M
"Model Non-Icing Surfaces for Cold-Climate Wind Turbines"
M. Brown(*ORNL*), M. Yamada (*GE*), IDC Innovation Award, *Comp. Phys. Comm*. (Aug. 2013)

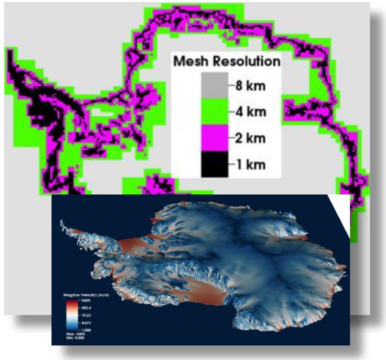




Smart Polymers, ALCF 50M
Subramanian Sankaranaran *(Argonne National Laboratory).* Fundamental understanding of stimuli response of smart polymers.

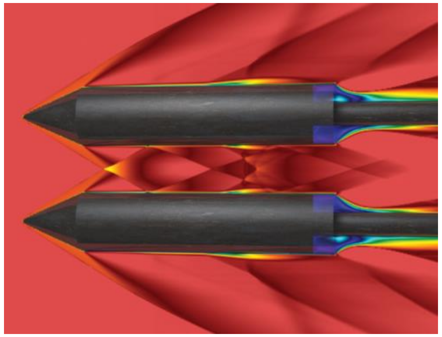
Solar Thermal Fuels, NERSC 30M
Jeffrey Grossman *(MIT).* Nanoscale template design for customizable solar thermal fuels for Concentrating Solar Power systems. *J. Chem Phys* 2013, v138





Ice Sheets, NERSC 13M
William Collins *(Lawrence Berkley National Laboratory).* Improve fidelity of global climate simulation ice sheet modeling; *Invited Speaker, American Geophysical Union Meeting* (2013)

Carbon Capture, OLCF 40M
Alan Grosvenor (*Ramgen Power Systems*) Accelerate design of shock wave turbo compressors for carbon capture and sequestration



Thank You

Individual Slides for Several Highlights

- **Carbon Capture**
  - Allan Grosvenor, Ramgen Power Technologies
- **Ice Nucleation**
  - M. Yamada, GE
- **Ice Sheet Modeling**
  - William Collins, Lawrence Berkley National Laboratory
- **Smart Polymers**
  - Subramanian Sankaranaran, Argonne National Laboratory
- **Solar Thermal Fuels**
  - Jeffrey Grossman, Massachusetts Institute of Technology

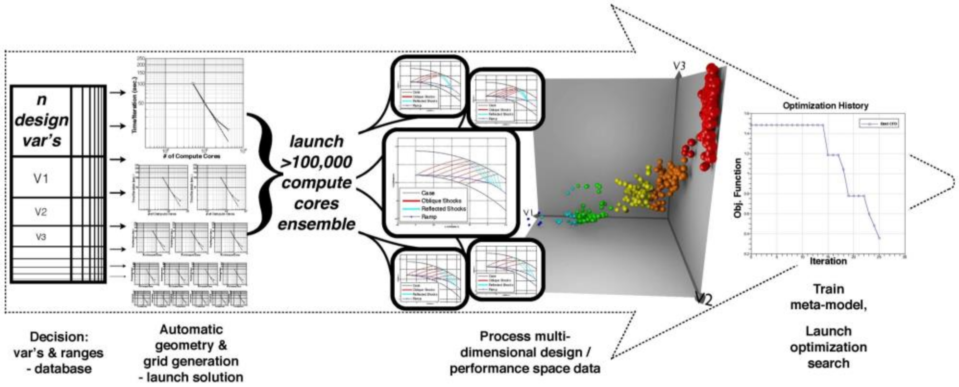
Turbo Compressor Innovation

Breakthrough aerodynamic design optimization

ALCC Project
Allan Grosvenor, Ramgen Power Systems
Allocated hours: 40M

Science Objectives and Impact

- Ramgen Power Systems is developing shock wave compression turbo machinery to meet DOE goals for reducing Carbon Capture and Sequestration (CCS) costs
- Complementary goal: design a gas turbine with dramatically lower costs and higher efficiency
- Compressing CO_2 to the required 100 atmospheres represents approximately 33 percent of the total cost of Sequestration



Leadership-scale ensemble runs on Jaguar support intelligently-driven design optimization

OLCF Contribution

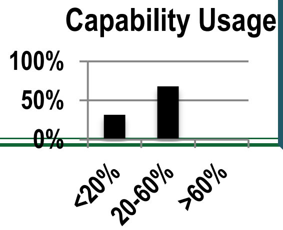
- 50x improvement in code scalability with more efficient memory utilization
- Accelerated I/O by 10x with optimizations and ADIOS
- Intelligent use of ensembles to explore parameter space using 240,000 cores

Results

- Transformed Ramgen's aerodynamic design process with a new data workflow for design optimization
- Observed designs with valuable new characteristics, from ensembles not possible without Jaguar
- Created a new workflow paradigm that accelerates design of compressors
- Accelerated computational design cycle for turbo machinery from months to 8 hours!

Non-Icing Surfaces for Cold Climate Wind Turbines

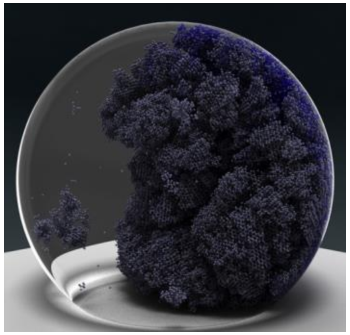
Molecular Dynamics Simulations



ALCC
Masako Yamada
GE Global Research
Hours used: 37,842.000

Science Objectives and Impact

- **Wind turbines, the fastest-growing source of electricity, are underused in cold climates, where ice on turbines reduces their efficiency and operational availability**
- **Reduce wind turbine downtime in cold climates by understanding the microscopic mechanism of water droplets freezing on surfaces**
- **Determine the efficacy of non-icing surfaces at different operation temperatures**



Location of ice nucleation varies dependent on temperature and contact angles. Visualization by M. Matheson (ORNL)

Performance & OLCF Contribution

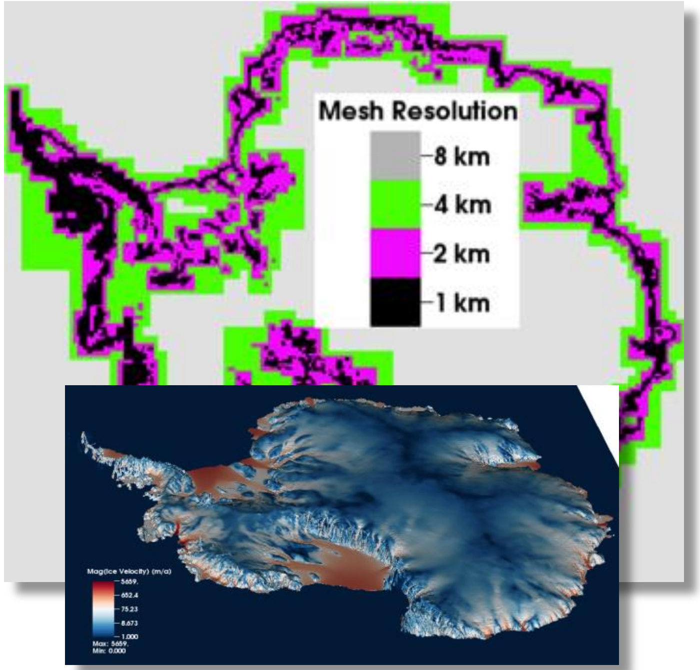
- OLCF/CAAR team prepared LAMMPS for use with GPUs on Titan
- OLCF extended LAMMPS GPU readiness to include 3-body forces, necessary for this project, achieved 5x speedup for this project
- As a result of effective use of GPUs, this project overachieved its original goals
- OLCF provided visualization services

Science Results

- Simulated ice formation within million-molecule water droplets on a variety of surfaces under isothermal and cooling conditions
- Replicated GE's experimental results and deepened the understanding of freezing at the molecular level
- Selected the mW interaction potential for water, resulting in a 40x speedup as compared to the SPC/E interaction originally envisioned for this project

Projections of Ice Sheet Evolution Using Advanced Ice and Ocean Models

- **Goal: Dramatically improve fidelity of global climate simulation ice sheet modeling; currently a large source of uncertainty in sea level predictions**
- **Completed: New BISICLES code with Adaptive Mesh Refinement allows high spatial resolutions needed for science; implemented an offline-coupling scheme between CISM-BISICLES and the POP2x ocean model**
- **Conducted the first large-scale, coupled ice sheet / ocean evolution simulations for Antarctica and the Southern Ocean; presented in an invited talk at the 2013 AGU meeting**

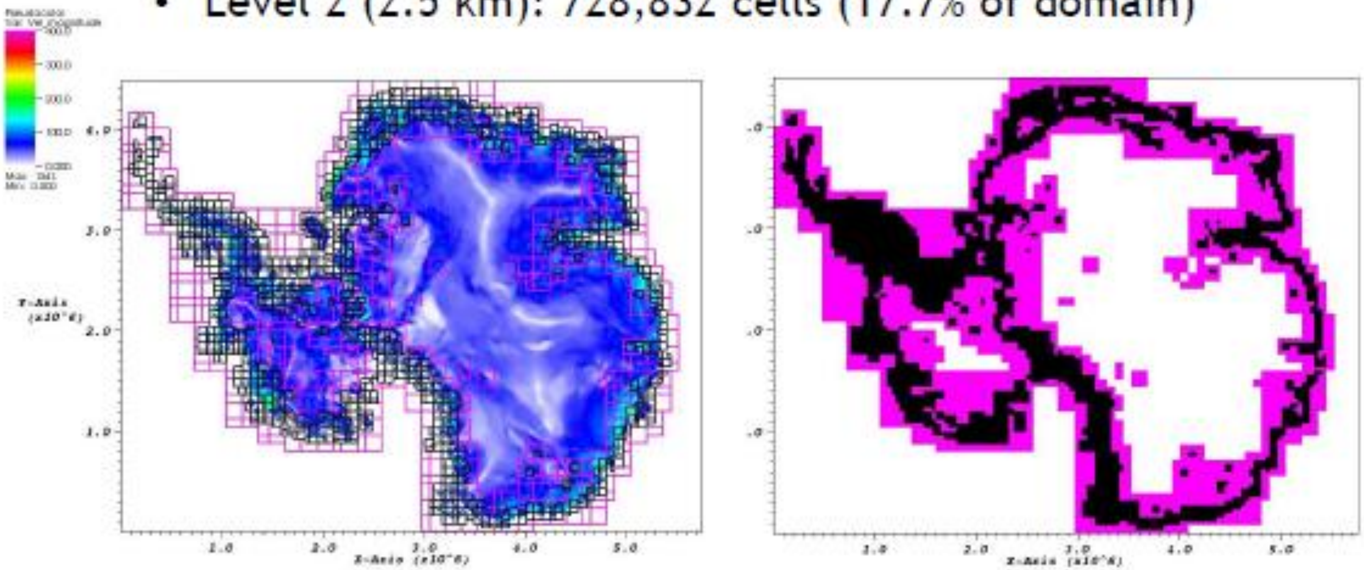


Results of a full-continent Antarctica simulation at 1-km resolution in equilibrium with initial conditions based on subshelf melt forcing from a POP2x model. Top: Distribution of mesh resolution for this problem. Bottom: Depth-averaged velocity from CISM-BISICLES draped over Antarctic ice sheet surface topography.

PI: W. Collins, LBNL
NERSC Repo m1343

Antarctica: Projections of Ice Sheet Evolution

- 10 km base mesh with 2 levels of refinement (5 km, 2.5 km)
  - base level (10 km): 258,048 cells (100% of domain)
  - level 1 (5 km): 431,360 zones (41.8% of domain)
  - Level 2 (2.5 km): 728,832 cells (17.7% of domain)



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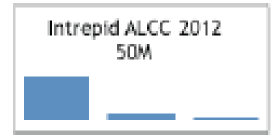
BISICLES

Los Alamos NATIONAL LABORATORY

University of BRISTOL

Smart Polymers for Drug Delivery

Subramanian Sankaranarayanan (PI), Argonne National Laboratory



Impact and Approach

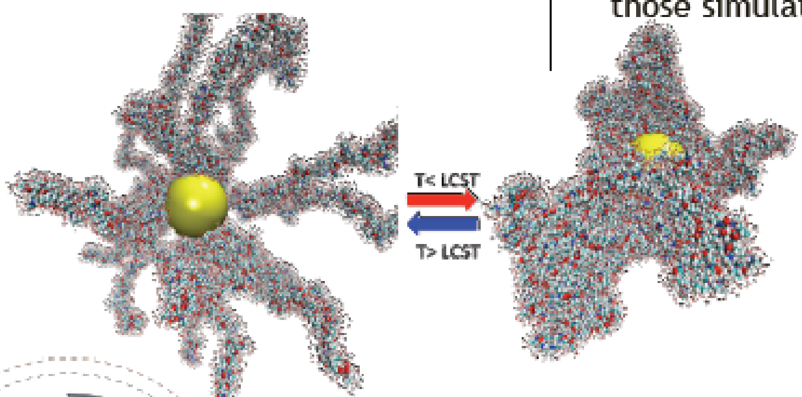
- Fundamental understanding of stimuli response of smart polymers
- Identify role of solvation in inducing phase transition
- Design of controlled drug delivery systems

Accomplishments

- **Identified the atomistic origin of coil-to-globule phase transition in thermosensitive polymers**
- Ordering of water molecules is shown to play a critical role in dictating the polymer conformation
- Experimentally probed polymer chains with degree of polymerization similar to those simulated on BG/P

ALCF Contributions

- ALCF recommended and built memory optimized version of NAMD for large scale computation.
- ALCF trained post-docs to use NAMD efficiently on Blue Gene/P (load balance parameters).
- ALCF fixed code that parsed input file and resolved a communication memory issue.

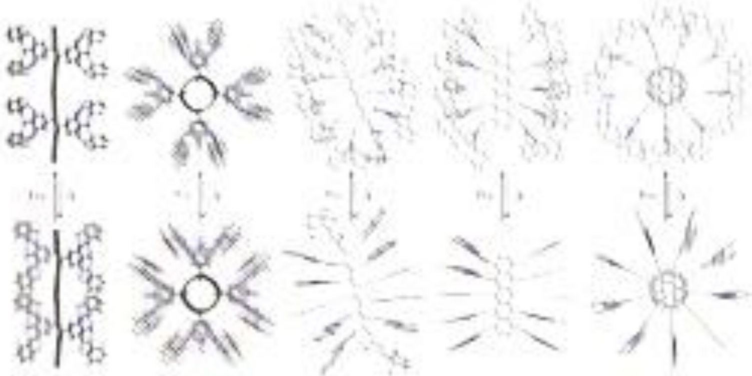


Expanded brush structure

Collapsed brush structure

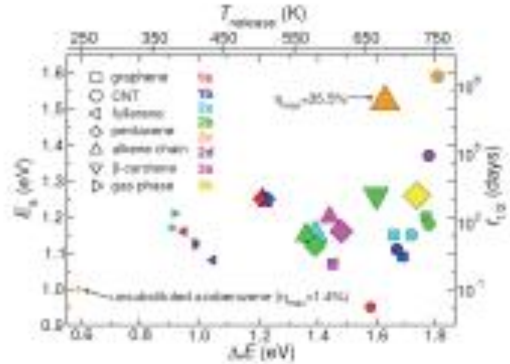
"The unique role of water in inducing a conformational transition of thermosensitive polymer from a coil to globule across its lower critical solution temperature was revealed through the ALCF allocation. Water molecules form an ordered structure around the polymer chains. Breaking of this cage acts as a precursor to the collapse. Computational modeling can allow researchers to identify ways of controlling the conformational dynamics and design efficient drug delivery systems (Argonne National Laboratory) "

First-Principles Design of Novel Solar Thermal Fuels

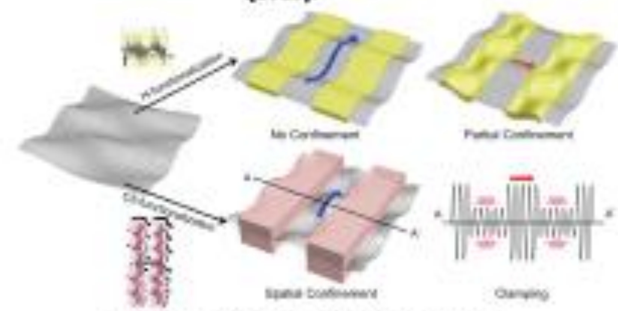


NERSC resources were used to:

- Design a nanoscale template/photoisomer platform (examples above) for customizable solar thermal fuels with a wide range of tunable properties:
  - energy density
  - thermal stability/lifetime
  - solar absorption efficiency
  - maximum temperature of released heat
- Identify structure-function relationships to guide choice of template & photoisomer for specific applications (top right).
- Understand heat transport mechanisms, that play a key role in conversion efficiency, for graphene-based fuels (right).



A. M. Kolpak and J. C. Grossman, J. Chem. Phys. 138, 034303 (2013).



J. Y. Kim, J.-H. Lee, and J. C. Grossman, ACS Nano 6, 9050 (2012).

ALCC Project (BES)
PI: J. Grossman (MIT)

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