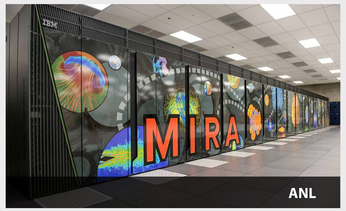
SciDAC on DOE's Leadership Computing Facility

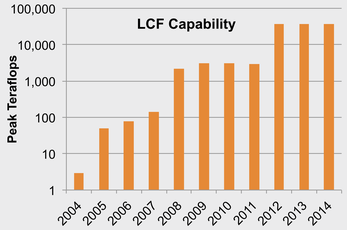
Mission of the LCF

What is the Leadership Computing Facility (LCF)?



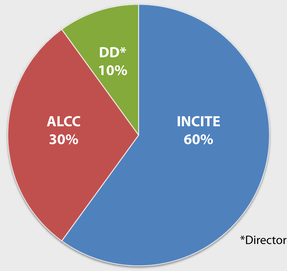
- Collaborative DOE Office of Science program at ORNL and ANL.
- Mission: Provide the computational and data resources required to solve the most challenging problems.
- 2-centers/2-architectures to address diverse and growing computational needs of the scientific community.
- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive 10x to 100x more resource than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).

We have increased our system capability by 10,000 times since our founding in 2004



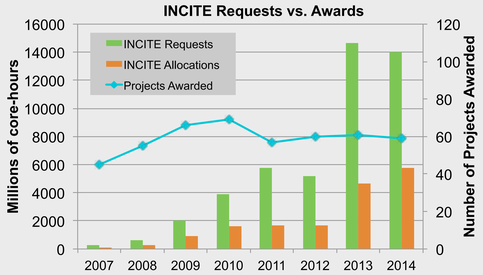
- Strong partnerships with computer designers.
- LCF users employ large portions of the machine for large fractions of time.
- We accomplished this through strong partnerships with our users to scale codes and algorithms.

Three primary ways for access to LCF
Distribution of allocable hours



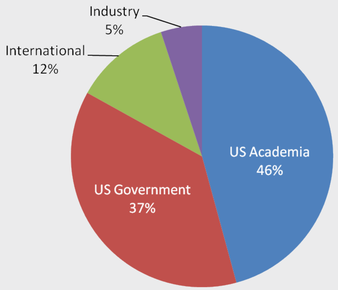
*Director's Discretion

Demand for INCITE resources exceeds supply with more time requested than available – Number of projects remains flat



2014 INCITE award statistics

PIs by Affiliation (Awards)

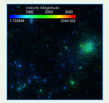
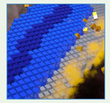
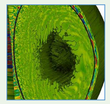


- Request for Information helped attract new projects.
- Total requests ~14 billion core-hours.
- Awards of 5.8 billion core-hours for CY 2014.
- 59 projects awarded of which 21 are renewals.

Acceptance rates
- 36% of nonrenewal submittals.
- 91% of renewals.

ORNL 2014-G00838/jbs

Science Achievements (including focus on SciDAC) on LCF

	Project	Science Objective	Science Result
	**Exploring the Nature of the Lightest Massive Particles in the Universe** Salman Habib *Argonne National Laboratory*	• To understand the distribution of mass in the universe, relevant to dark energy, dark matter, and other areas of astrophysics research. • To create synthetic cosmological surveys that can support analysis of observational data. • To simulate cosmic structure using a highly scalable application with a multi-algorithmic structure.	• Precision study of effects of massive neutrinos on cosmological structure formation. • Synthetic sky catalog with the latest cosmological parameters as determined by Planck and other observational surveys.
	**Lattice QCD: Spectrum and Properties of Exotic Mesons** Paul Mackenzie *Fermilab*	• Establish theoretical capability to predict the existence of new particles. • Predict new discoveries from experiments at the Continuous Electron Beam Accelerator Facility at JLab following the 12GeV upgrade. • Predict the spectrum of exotic mesons generated by the excitation of the gluonic field binding the quarks.	• Unprecedented determination of the ρ meson resonance using LQCD. • Demonstrated the methodology for determining resonance properties, enabling future calculations of exotic mesons.
	**Nuclear Physics: The Limits of the Nuclear Landscape** James Vary *Iowa State University*	• Identify how protons and neutrons can be bound within a nucleus and the nuclear drip lines denoting the end of nuclear binding. • Uses ranging from potential cancer treatments to a better understanding of superconductivity.	• Identify how many protons and neutrons can be bound within a nucleus. • Identify the nuclear drip lines that denote the end of nuclear binding. • Project represents at step toward "designer nuclei," with uses ranging from potential cancer treatments to a better understanding of superconductivity.
	**The Bleeding 'Edge' of Fusion** CS Chang *Princeton Plasma Physics Laboratory*	• Fusion efficiency of ITER to be determined by edge plasma transport. • First-principles simulation of edge physics on Titan. • Predictions validated. New insight gained through analysis of results. Success with DIII-D plasma simulations.	• Simulated nonlinear coherent turbulence structures. • Identified the momentum source and its inward transport process and predicted the divertor heat load distribution. • All for the first time in first-principles calculations of a tokamak reactor.

SciDAC-Affiliated Projects at LCF:

2013

Title	PI Name	Institution	OLCF Hrs (millions)	ALCF Hrs (millions)
Computing the Dark Universe	Salman Habib	Argonne	0	40
High-Fidelity Simulation of Tokamak Edge Plasma Transport	C.S. Chang	PPPL	100	0
Lattice QCD	Paul Mackenzie	Fermi	140	430
Nuclear Structure and Nuclear Reactions	James Vary	Iowa State U	74	81
Performance Evaluation and Analysis Consortium (PEAC) End Station	Lenny Oliker	LBNL	45	40
Precision Many-Body Quantum Simulations of Functionalized Structures	Shiwei Zhang	W&M	27	0
Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and Lifetime	Brian Wirth	Oak Ridge	5	7.5
High-Resolution Coupled Climate Simulations on Titan with GPU Acceleration	Mark Taylor	Sandia	64	0
Projections of Ice Sheet Evolution	Stephen Price	LANL	2.6	0
		TOTAL	458	598

Acknowledgements:
LCF Vendor Partners: IBM, Cray, AMD, NVIDIA, etc.
LCF Users: DOE ASCR Leadership Computing Program

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2014

Title	PI Name	Institution	OLCF Hrs (millions)	ALCF Hrs (millions)
Lattice QCD	Paul Mackenzie	Fermi	100	240
High-Fidelity Simulation of Tokamak Edge Plasma Transport	C.S. Chang	PPPL	129	100
Cosmological Simulations for Large-scale Sky Surveys	Salman Habib	Argonne	100	100
Nuclear Structure and Nuclear Reactions	James Vary	Iowa State U	104	100
High-Resolution Coupled Climate Simulations on Titan with GPU Acceleration	Mark Taylor	Sandia	100	0
Performance Evaluation and Analysis Consortium (PEAC) End Station	Lenny Oliker	LBNL	45	30
QMC Simulations DataBase for predictive modeling and theory	David Ceperely	UIUC	100	100
Precision Many-Body Quantum Simulations of Functionalized Structures	Shiwei Zhang	W&M	30	0
Assembling and sustaining the acid mantle of the human skin barrier	Michael Klein	Temple U	75	0
Correlated Electrons in Photoactive and Superconducting Materials	Lucas Wagner	UIUC	0	60
Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An Ab Initio Study of Liquid Water	Robert DiStasio	Princeton U	0	350
The Spectrum and Properties of Exotic Mesons in Quantum Chromodynamics	Robert Edwards	Jefferson Lab	250	0
Cosmic Frontier Computational End-Station	Salman Habib	Argonne	0	100
Understanding Helium Plasma Mediated Tungsten Surface Response to better predict Fusion Plasma Facing Component Performance in	Brian Wirth	U Tennessee	30	66
Hypernuclei and Charmed Nuclei	Martin Savage	U Washington	65	0
		TOTAL	1128	1246