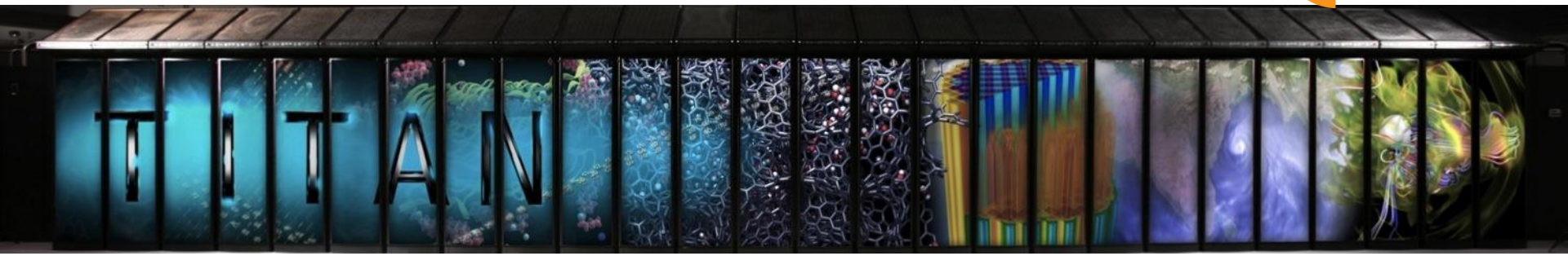
An Overview of the Oak Ridge Leadership Computing Facility

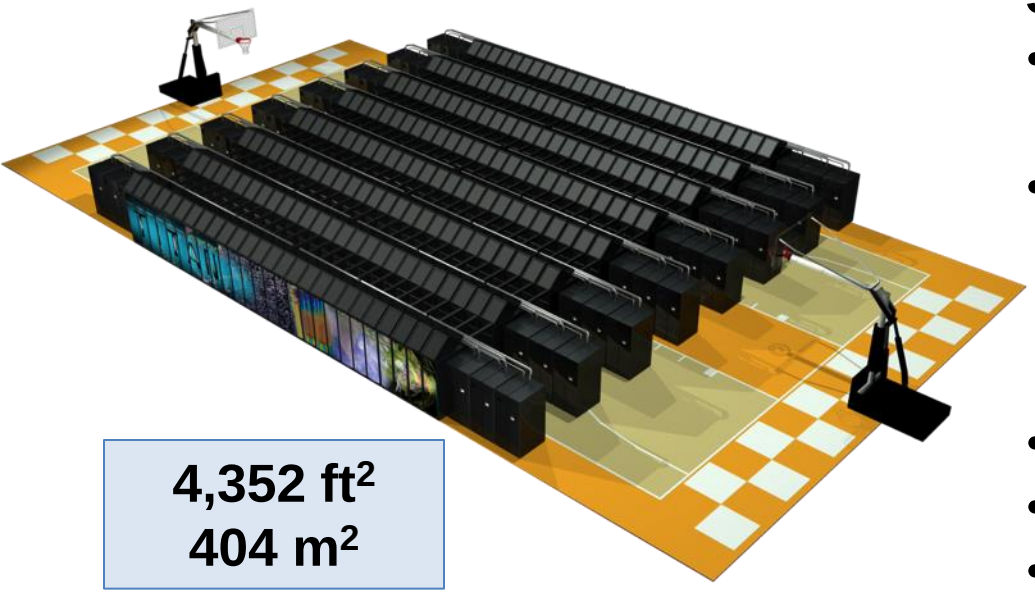
Presented by:
Judith Hill
Task Lead for Scientific Computing Liaisons
Oak Ridge Leadership Computing Facility (OLCF)
National Center for Computational Sciences (NCCS)

CSGF Program Review: HPC Workshop
July 17, 2014
Washington, DC

ORNL's "Titan" Hybrid System: The Nation's Most Powerful Computer

#2 TOP500® SUPERCOMPUTER SITES





4,352 ft²
404 m²

SYSTEM SPECIFICATIONS:

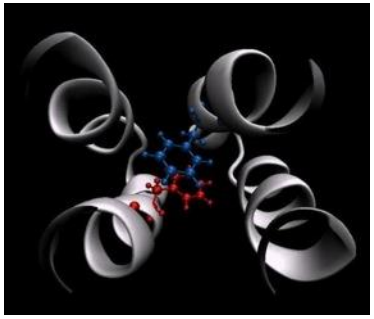
- Peak performance of 27.1 PF
  - 24.5 GPU + 2.6 CPU
- 18,688 Compute Nodes each with:
  - 16-Core AMD Opteron CPU
  - NVIDIA Tesla "K20x" GPU
  - 32 + 6 GB memory
- 512 Service and I/O nodes
- 200 Cabinets
- 710 TB total system memory
- Cray Gemini 3D Torus Interconnect
- 8.9 MW peak power

OAK RIDGE National Laboratory

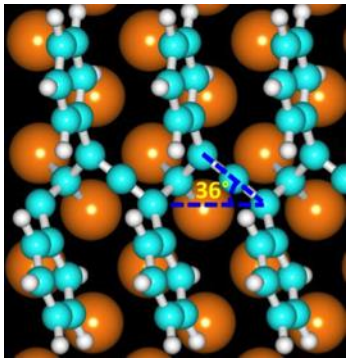
High-impact science across a broad range of disciplines

For example in 2013:

Paleoclimate Science
"Northern Hemisphere forcing of Southern Hemisphere climate during the last deglaciation,"
Feng He (UW Madison), *et al*., *Nature*, February (2013)

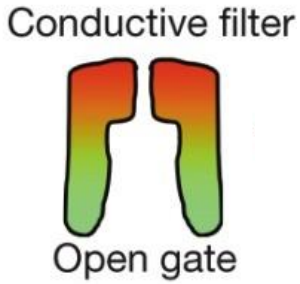


Molecular Biology
"A phenylalanine rotameric switch for signal-state control in bacterial chemoreceptors"
D. Ortega (UTK),
Nature Communications
December (2013)

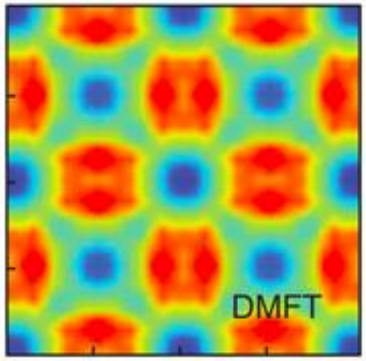


Polymer Science
"Self-Organized and Cu-Coordinated Surface Linear Polymerization"
Qing Li, B. Sumpter (ORNL),
Nature Scientific Reports.
July (2013)

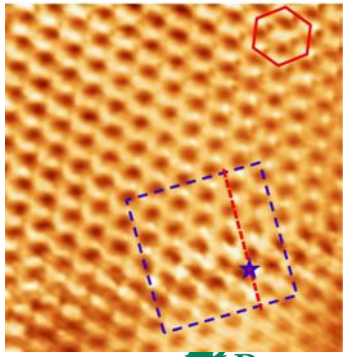
Molecular Biology
"Recovery from slow inactivation in K1 channels is controlled by water molecules"
Jared Ostmeyer, et al. (U. Chicago) *Nature*, Sept. (2013)



Superconductivity
"Doping dependence of spin excitations and correlations with high-temperature super-conductivity in iron pnictides,"
Meng Wang(IOP CAS Beijing),
Nature Communications.
December (2013)



Complex Oxide Materials
"Atomically resolved spectroscopic studyof Sr2IrO4: Experiment and theory," Qing Li (ORNL), E.G. Eguiluz (UTK)
Nature Scientific Reports.
October (2013)

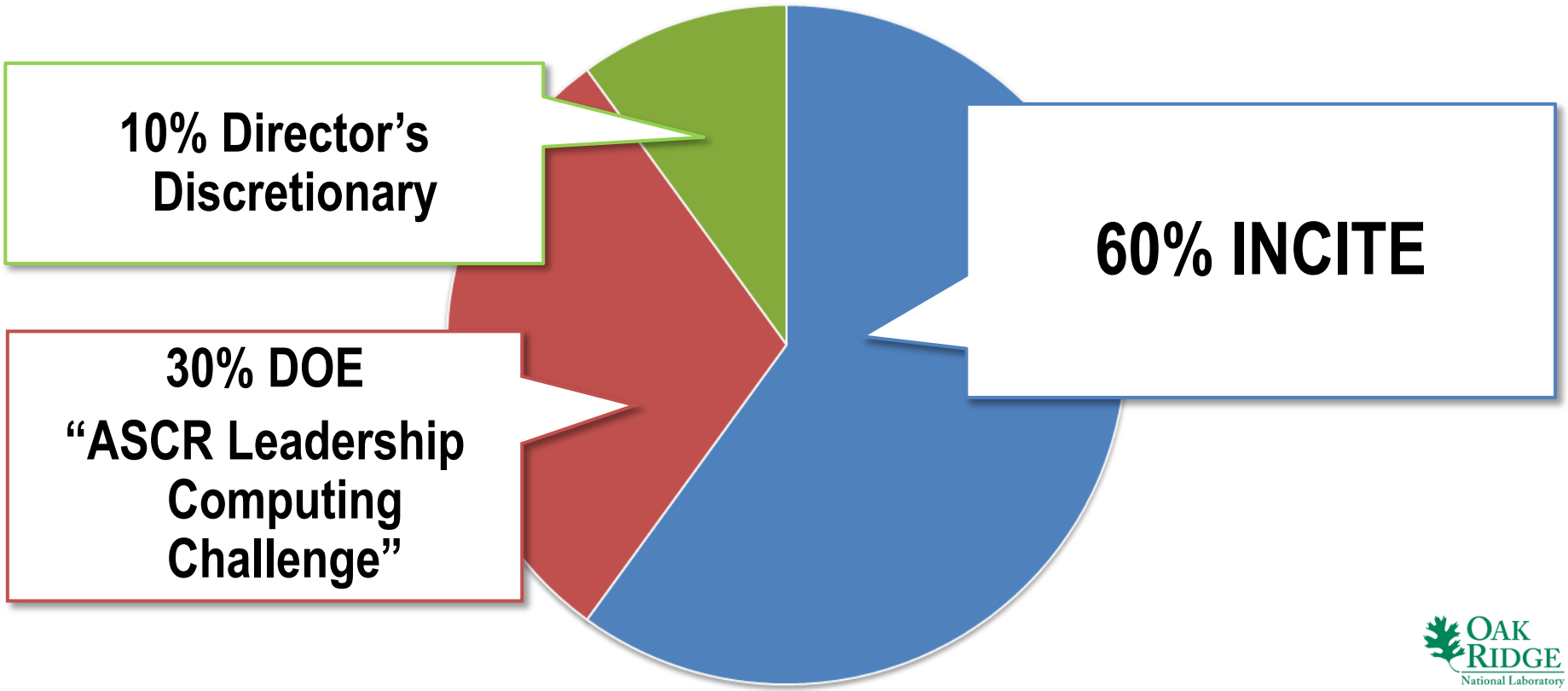


RIDGE National Laboratory

DOE Computational Facilities Allocation Policy for Leadership Facilities

Primary Objective:

- *"Provide substantial allocations to the open science community through an peered process for a small number of high-impact scientific research projects"*



OLCF allocation programs
Selecting applications of national importance

	60% INCITE		30% ALCC		10% Director's Discretionary	
Mission	High-risk, high-payoff science that requires LCF-scale resources		High-risk, high-payoff science aligned with DOE mission		Strategic LCF goals	
Call	1x/year – (Closes June)		1x/year – (Closes February)		Rolling	
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical Size	30 - 40 projects	20M - 150M core-hours/yr.	10 - 20 projects	10M – 75M core-hours/yr.	100s of projects	500K – 3M core-hours
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed by	INCITE management committee (ALCF & OLCF)		DOE Office of Science		OLCF management	
Availability	Open to all scientific researchers and organizations including industry					

What is INCITE?

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

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.

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

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

ALCC

- ASCR Leadership Computing Challenge
- Awards ~30% of time at OLCF
- Emphasis on high-risk, high-payoff simulations in areas directly related to DOE's energy mission

http://science.energy.gov/ascr/facilities/alcc/

OLCF Director's Discretion

- Opportunity to enhance scalability and productivity of scientific codes
- Preparation for INCITE or ALCC

https://www.olcf.ornl.gov/support/documents-forms/

CSGF Allocation Program

- Subset of DD time specifically for CSGF fellows
- Only CSGF fellows can use the allocation for their own research
- Review process differs from usual DD

Relevant links

INCITE Program
http://www.doeleadershipcomputing.org/

ALCC
http://science.energy.gov/ascr/facilities/alcc/

Oak Ridge Discretionary Program
https://www.olcf.ornl.gov/support/documents-forms/

Contacts

For details about the INCITE program:

www.doeleadershipcomputing.org
INCITE@DOEleadershipcomputing.org

For details about the OLCF:

www.olcf.ornl.gov
help@nccs.gov, 865-241-6536

Contact Me:

Judith Hill, hilljc@ornl.gov, 865-576-8453

Questions?