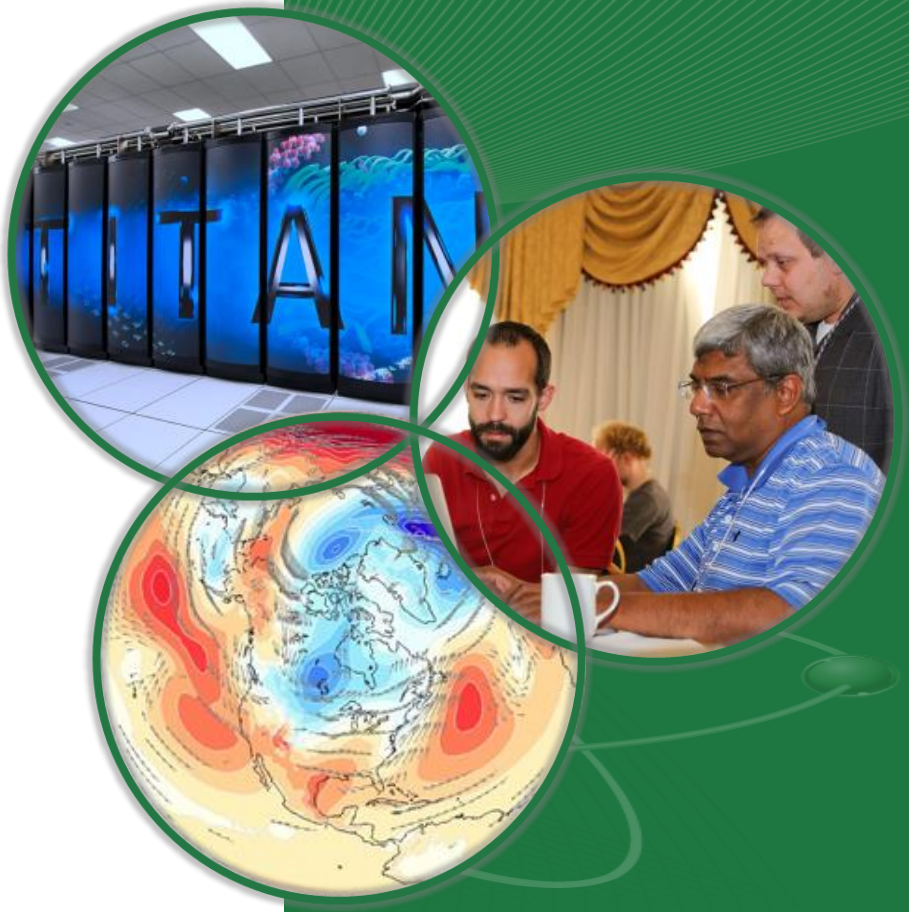
2014 Year in Review



Jack Wells

Director of Science

Presented to:

OLCF Users' Group Meeting

June 24, 2015

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory | OAK RIDGE LEADERSHIP COMPUTING FACILITY

2014: A Year of Superlatives for OLCF

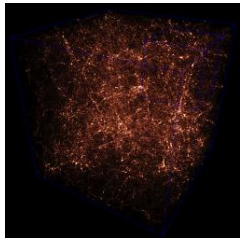
- More publications in “high-impact”* journals than ever before
- Highest-yet survey rating on overall satisfaction (4.6/5),
- Maximizing both capability usage and utilization!
  - Largest percentage of capability† usage (62.6%),
  - Greatest number of core-hours delivered to projects (4.2B),
  - Extremely high utilization rate (89.6%)

*15 pubs in journals with impact factor of 9 or above
†Capability jobs use 20% or more of the compute nodes

Science Accomplishments Highlights

All from 2014 INCITE Program on Titan

Cosmology



Salman Habib
Argonne National Laboratory

Habib and collaborators used its HACC Code on Titan's CPU–GPU system to conduct today's largest cosmological structure simulation at resolutions needed for modern-day galactic surveys.

K. Heitmann, 2014. *arXiv.org,* 1411.3396

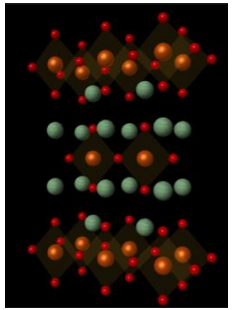
Combustion

Jacqueline Chen
Sandia National Laboratory

Chen and collaborators for the first time performed direct numerical simulation of a jet flame burning dimethyl ether (DME) at new turbulence scales over space and time.

A. Bhagatwala, et al. 2014. *Proc. Combust. Inst.* **35**.

Superconducting Materials



Paul Kent
ORNL

Paul Kent and collaborators performed the first ab initio simulation of a cuprate. They were also the first team to validate quantum Monte Carlo simulations for high-temperature superconductor simulations.

K. Foyevtsova, et al. 2014. *Phys. Rev. X* **4**

Molecular Science

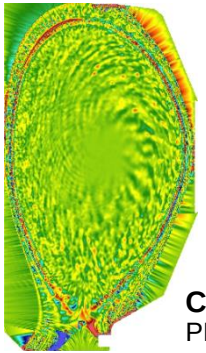
Michael Klein
Temple University

Researchers at Procter & Gamble (P&G) and Temple University delivered a comprehensive picture in full atomistic detail of the molecular properties that drive skin barrier disruption.

M. Paloncyova, et al. 2014. *Langmuir* **30**

C. M. MacDermaid, et al. 2014. *J. Chem. Phys.* **141**

Fusion



C.S. Chang
PPPL

Chang and collaborators used the XGC1 code on Titan to obtain fundamental understanding of the divertor heat-load width physics and its dependence on the plasma current in present-day tokamak devices.

C. S. Chang, et al. 2014. *Proceedings of the 25th Fusion Energy Conference, IAEA*, October 13–18, 2014.

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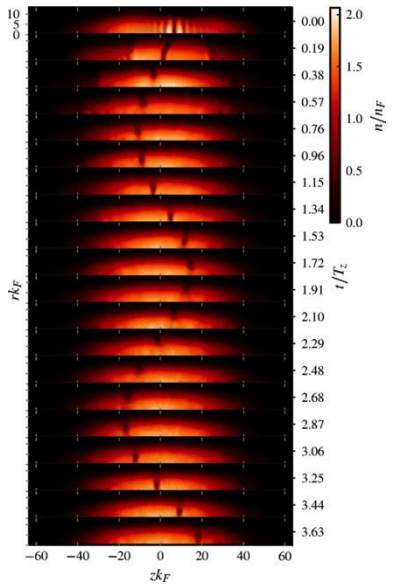
CY 2014 OLCF Publication Product is Strong

More publications in “high-impact” journals than ever before.

Confirmed Peer-Reviewed Publications	229
User only papers	183
Joint User & Staff papers	26
Staff only papers	20

Articles in High-Impact Publications (ISI Journal Impact Factor)

1 Nature (JIF: 42)	4 Science (JIF: 31)	1 Chem. Soc. Rev. (JIF: 30)
1 Acc. Chem. Res. (JIF: 24)	1 Nature Physics (JIF: 21)	1 ACS Nano (JIF: 12)
2 Astrophys. J Suppl. S. (JIF: 14)	1 JACS (JIF: 11)	1 Nature Comm. (JIF: 11)
2 PNAS (JIF: 10)	1 Phy. Rev. X (JIF: 8)	10 Phys. Rev. Lett. (JIF: 8)



Time-dependent oscillations of a vortex ring of unitary Fermi gas in an elongated harmonic trap. time-reversal invariance using the Titan supercomputer.

Aurel Bulgac, et al. (2014). Physical Review Letters **112**

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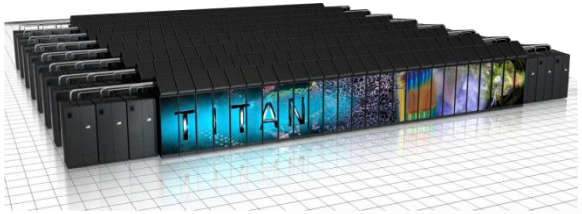
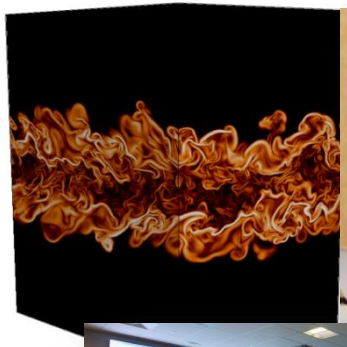
The OLCF's mission is to enable breakthrough science by:

- Fielding the most powerful capability computers for scientific research,
- Building the required infrastructure to facilitate scientists' use of these computers,
- Selecting a few time-sensitive problems of national importance that can take advantage of these systems, and
- Partnering with these teams to deliver breakthrough science.



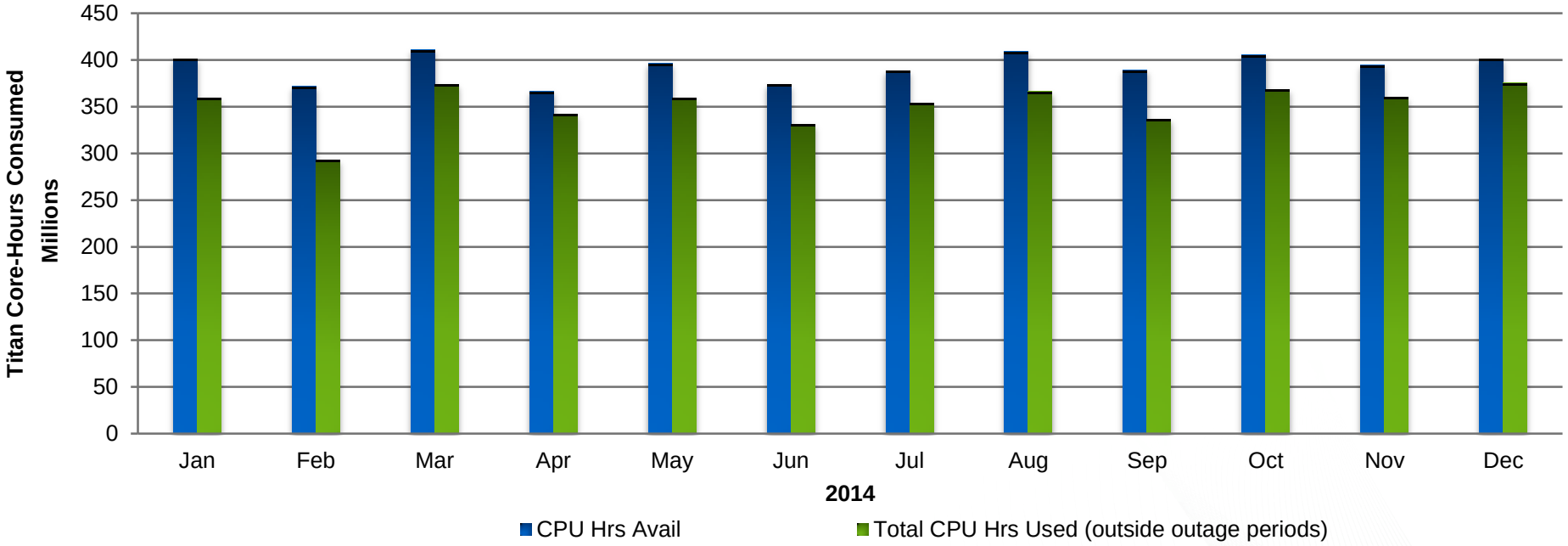


Fielding the most powerful capability computers

- **Titan is very productive**
  - #1 system when delivered in Nov. 2012, #2 since
  - Very high capability use & overall usage
  - Typical early life stability problems resolved. Preventive maintenance in 2013 on node boards has resulted in excellent uptime and more delivered hours than ever before

- **Contract for Summit signed**
  - 5-10x more powerful than Titan on applications will be among the world's most powerful
  - Delivery in 2017-2018

Titan System Utilization – 89.63% in CY14



The consistently busy Titan system delivered more than 350M hours/month and 4.2B of 4.7B available hours.
- Very high system utilization for a capability machine/workload: 89.63% -

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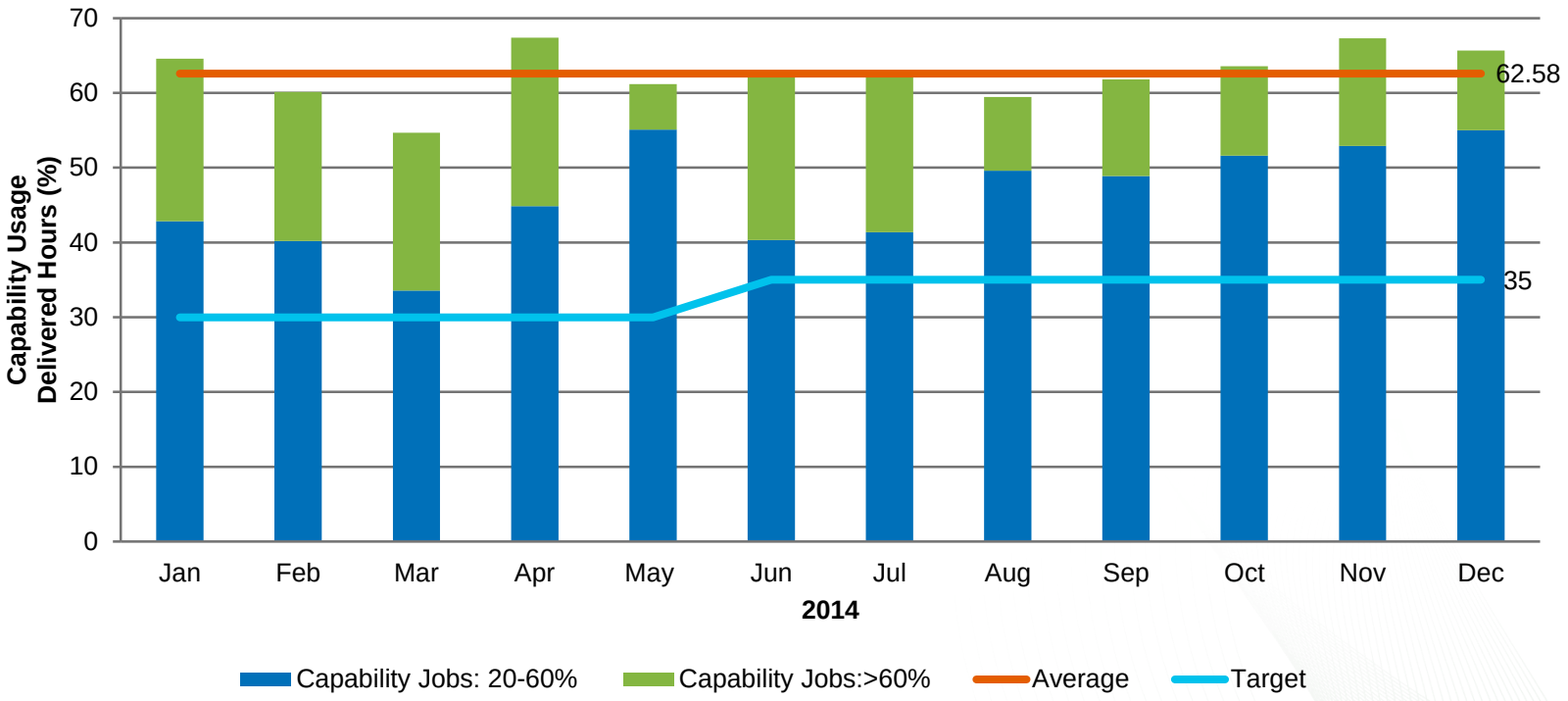
Capability Usage for Large/Largest Jobs



OLCF queue policy additionally rewards jobs using 60+% of the nodes. Positive impact to overall capability usage

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Building the required infrastructure

- **Data Management**
  - External FS (late 2013): 32 PB capacity and 1 TB bandwidth.
  - HPSS: 2 PB of disk cache and 20 GB/s of bandwidth. RAIT (2014). 53M files / 44 PB
  - Key leadership roles in HPC community
    - Board of Directors, OpenSFS Lustre group. (Chair, 2013-2014)
    - HPSS Executive Committee and Funding for 4 HPSS developers.

- **Data Analytics and Visualization**
  - Significant upgrade to EVEREST visualization laboratory (2014)
  - Data analytics cluster refresh (2014)
  - Implemented “Data Liaisons” to assist data and workflow needs
  - New **Advanced Data and Workflows Group** to help users understand results and get the most from systems. (2015)
  - 7 DOE science data pilot projects at SC’14
  - Prototyped ‘graphics mode’ on Titan, allowing GPUs to directly support visualization (2015 introduction)
- **Networks**
  - 100Gb/s connection to ESnet
  - High performance data transfer nodes

2015 Rhea Upgrade

- **Mission: Provide a conduit for large-scale scientific discovery via pre/post processing and analysis of simulation data generated on Titan.**

Rhea, the Dell analysis cluster, has 512 nodes.

- **Compute Resources:**
  - Each of the 512 (+ 4 spare) compute nodes is a Dell PowerEdge C6220 featuring dual Intel® Xeon® E5-2650 CPUs and **128** GB of RAM. Each CPU features (8) physical cores running at 2.0 GHz, for a total of (16) physical cores.
  - 8 nodes with two Intel® Xeon® CPUs running at 2.3 GHz , **1** TB of RAM and 2 K80 GPUs.
  - Rhea features a 4X FDR Infiniband interconnect.

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National Center for Computational Sciences
Oak Ridge Leadership Computing Facility

J. Hack, Director

L. Gregg, Division Secretary

OLCF Project Director – *A. Bland*
Deputy Project Director – *J. Whitt*
A. Barker, Training & Support Development
D. Bernholdt, Programming Environment and Tools
B. Hammontree, Facility Upgrades
J. Whitt, Project Management
J. Rogers, System Acceptance
K. Thach, Computer Infrastructure, Services, and Integration
J. Rogers, System Acquisition
T. Straatsma , Application Readiness
S. Oral – Storage System Evaluation

CCSD Asso. Projs. Director
K. Boudwin

Chief Technology Officer
A. Geist

Industrial Partnerships
S. Tichenor

Director of Science – *J. Wells*
Director, Computing & Facilities – *J. Rogers*
Operations Manager – *S. McNally*
INCITE Program Manager– J. Hill

Computer Science Research[5]

D. Bernholdt
C. Sonewald

S. Boehm[8]
M. Brim
N. Forington[6]
M. Gorentla-Venkata
O. Hernandez
T. Janjusic[7]
T. Jones
C. Kartsaklis
T. Naughton
P. Shamis
G. Vallee
J. Vasnier[6]
F. Winkler[6]

Advanced Data and Workflows

J. Hack [A]
L. Gregg [A]

V. Anantharaj
J. Daniel
J. Harney
B. Hernandez Arreguin
S. Klasky[5]
M. Matheson
N. Podhorszki[5]
D. Pugmire[5]
B. Smith
D. Stansberry

User Assistance & Outreach

A. Barker
S. Mowery

A. Carlyle
A. DiGirolamo
F. Foertter
R. French
C. Fuson
B. Gajus[5]
J. Gary
S. Parete-Koon
L. Rael
S. Ray
B. Renaud
D. Rose
J. Rumsey[1]
A. Simpson
J. Smith[5]
S. Stiles
V. Vergara-Larrea
R. Whitten[3,5]

Technology Integration

S. Vazhkudai
S. Mowery

S. Atchley
T. Barron
M. Griffith
R. Gunasekaran
S. Gupta[7]
Y. Kim
R. Miller
S. Oral[#]
H. Sim[8]
J. Simmons
D. Steinert
D. Tiwari
C. Wang
F. Wang
V. White
C. Zimmer

Scientific Computing

T. Straatsma
P. Ticknor

M. Berrill
M. Chen[7]
E. D'Azevedo[5]
M. Eisenbach
J. Hill [#]
A. Hynninen
W. Joubert
S. Laosooksathit[7]
J. Larkin[^]
Y. Li
D. Liakh
B. Messer
M. Norman
G. Ostrouchov[5]
T. Papatheodore
D. Rosenberg
R. Sankaran
A. Tharrington
A. Vose[4]

High-Performance Computing Operations

K. Thach
S. Allen

R. Adamson
J. Anderson
M. Bast
J. Becklehimer[4]
K. Bivens
B. Caldwell
M. Campfield
C. Cooper[1]
P. Curtis
A. Enger[4]
C. England
J. Evanko[4]
M. Ezell
A. Funk[4]
R. Gainey[1]
D. Garman[4]
E. Gershman
M. Gyurgyik
J. Hanley
J. Hill
J. Kincl
S. Koch
D. Leverman
J. Lewis[4]
D. Londo[4]
V. Martin
D. Maxwell[@]
M. McDonough[4]
Q. Mitchell
P. Newman
D. Pelfrey
R. Ray
A. Sachitano[4]
S. Shpanskiy
B. Sparks
L. Sorrillo
B. Tennessen[4]
S. White
C. Willis[4]

[1]Intern/Student
[2]Post Graduate
[3]JICS
4 Vendor-Cray, Inc.
[5]Matrixed
[6]Subcontractor
[^]Vendor –NVIDIA
* Interim
[7] Post Doc
[8] Post Master
[9] Post Bachelors
[#] Task Lead
[@] Technical Coordinator
[A] Acting

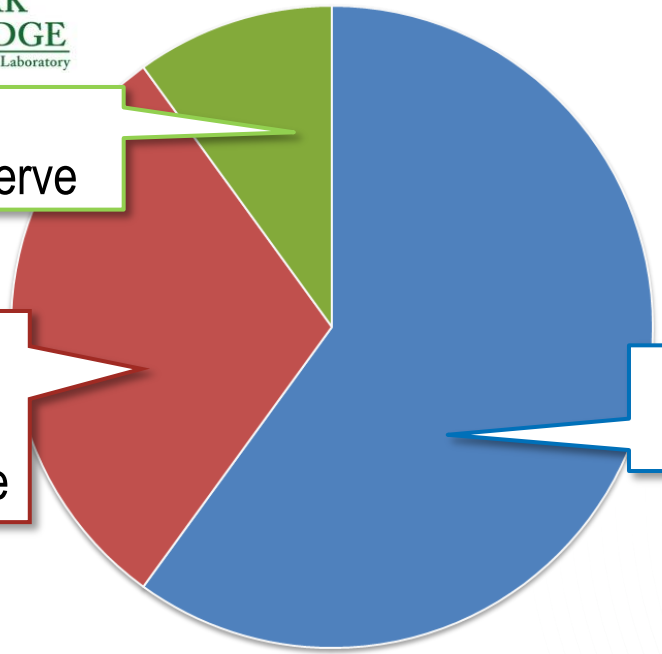
05/18/2015

OLCF allocation programs: Selecting applications of national importance

	INCITE – 60% of core-hrs		ALCC – 30% core-hrs		Director's Discretionary – 10%	
Mission	High-risk, high-payoff science that requires LCF-scale resources		High-risk, high-payoff science aligned with DOE mission		Strategic LCF goals	
Frequency and allocation year	1x/year January - December		1x/year July - June		Rolling	
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical Size	30 - 40 projects	16M - 150M core-hours/yr. (2014 avg-78M)	20 - 30 projects	2M – 75M core-hours/yr. (2014 avg-49M)	~140 projects	10K – 3M core-hours (2014 avg-4.4M)
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review		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					

Three primary user programs for access to LCF

Distribution of allocable hours



10% Director's Discretionary Reserve

30% ALCC

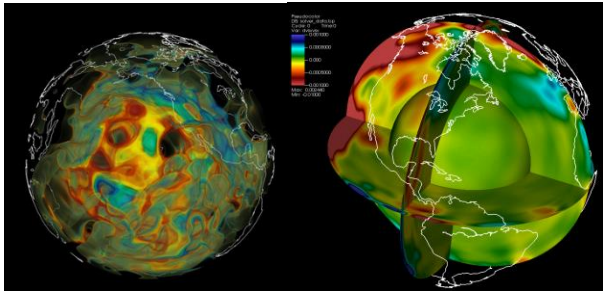
ASCR Leadership Computing Challenge

60% INCITE

Partnering with our users to deliver breakthrough science

- Developed Liaison model for user interaction with the facility
  - Computational, Data, Visualization
  - “Whatever it takes” to get the job done
  - Center for Accelerated Application Readiness
- User Assistance & Outreach group
  - Help users with routine and complex problems
  - Manage user agreements and accounts
  - Create web site, documentation, training including Hackathon
  - Responsible for outreach to DOE, users, and the general public

SPECFEM3D - visualization



Jeroen Tromp (Princeton) INCITE: Simulating global and regional seismic wave propagation

OLCF Liaison Contributions:

- Implemented the enormous I/O requirements of the code using the ADIOS middleware library for both input and output
- Developed a parallel reader for the VisIt visualization tool to enable more efficient analysis
- Optimized the parallel reader and provided new functionality to the science team

Judy Hill

Dave Pugmire

Norbert Podhorszki

User Support Metrics

The OLCF exceeded all targets for the User Results metrics in 2014.

Metric	Target	2013 Actual	2014 Actual
Overall OLCF Satisfaction score on the user survey.	3.5/5.0	4.4/5.0	4.6/5.0
Show improvement on results that scored below satisfactory in the previous period.	Results will show improvement in at least ½ of questions that scored below 3.5 in the previous period.	No question scored below satisfactory (3.5/5.0) on the 2014 survey.	No question scored below satisfactory (3.5/5.0) on the 2014 survey.
OLCF survey results related to problem resolution.	3.5/5.0	4.4/5.0	4.6/5.0
Percentage of user problems addressed within 3 business days.	80%	92%	90%
Average of all user support services ratings.	3.5/5.0	4.4/5.0	4.6/5.0

Director's Discretionary (DD) Reserve Time is Managed to Achieve Three Goals to Advance DOE's Mission

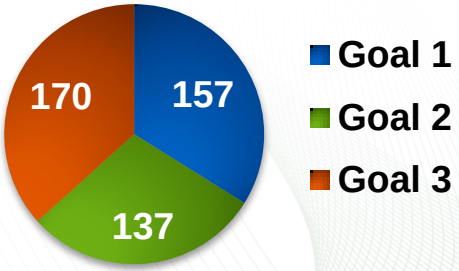
All DD proposals are peer-reviewed for quality and feasibility by ORNL researchers.

The goals of the Director's Discretionary (DD) program are threefold:

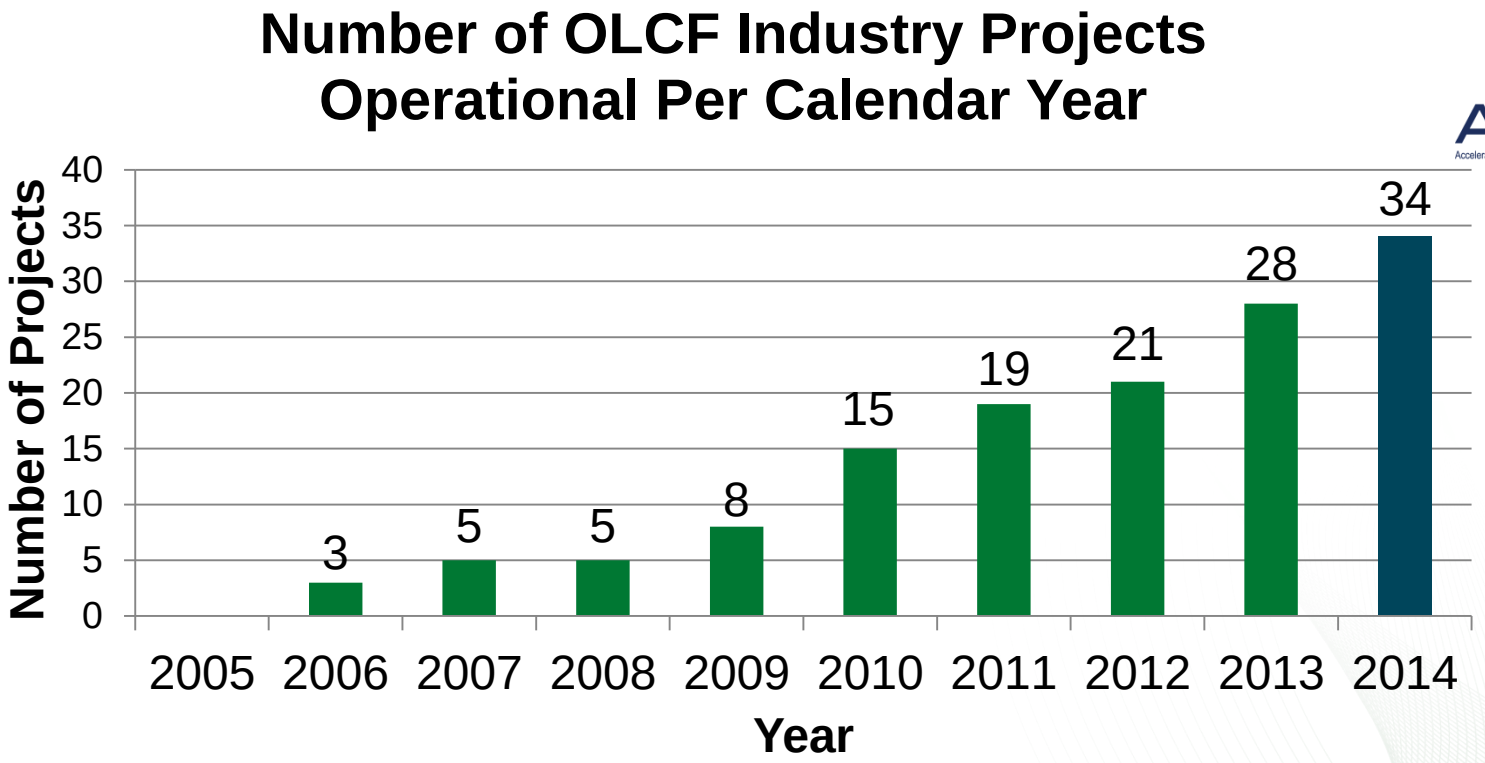
1. **Help prepare any user or potential user for leadership computing programs (INCITE & ALCC),**
2. **Broaden the community of researchers capable of using leadership computing, and**
3. **Develop R&D partnerships, both internal and external to ORNL, to advance DOE and ORNL strategic agendas.**

	Number of Projects	Titan Core Hours Used in 2014
Total Projects	173	464 Million
Subtotal Goal 1	65	157 Million
Subtotal Goal 2	42	137 Million
Subtotal Goal 3	66	170 Million

DD Time Used by Goal (M Core-Hours)



Industrial Partnerships:
Accelerating Competitiveness through Computational Sciences



Questions