

# Oak Ridge Leadership Computing Facility (OLCF) – Overview and Recent Activities

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Leadership Computing Facility

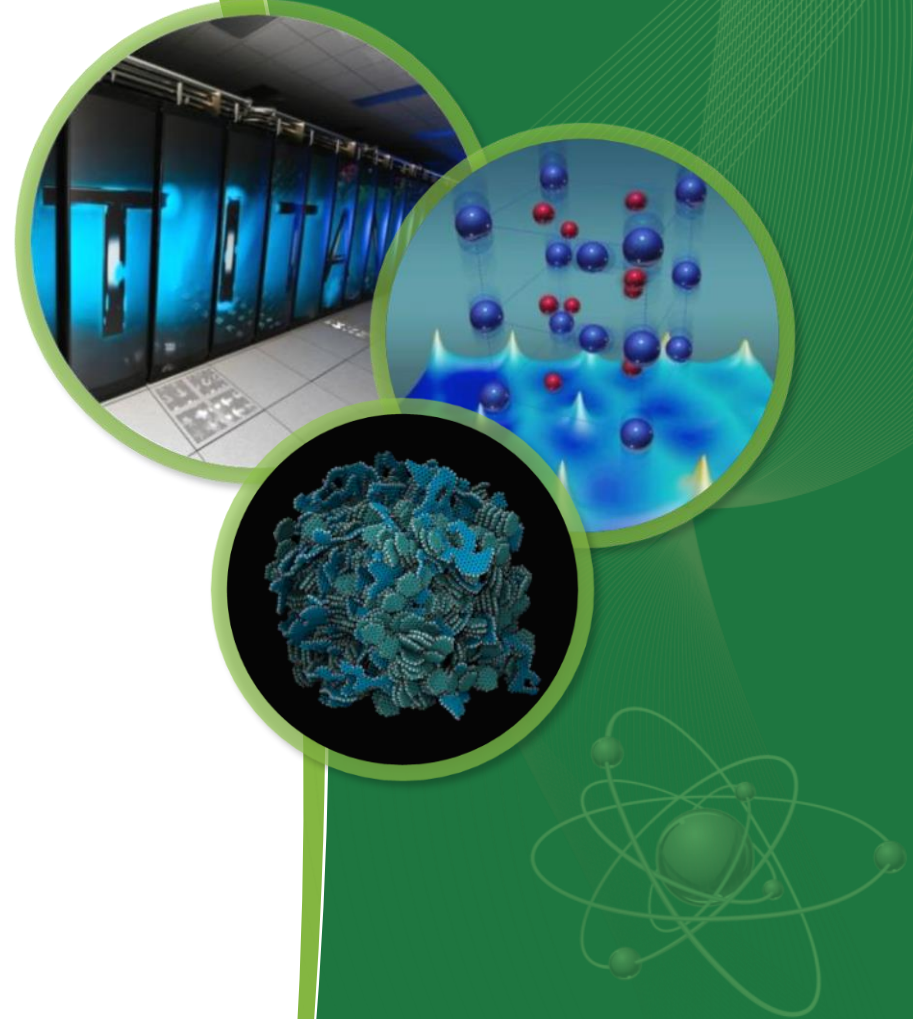
Oak Ridge National Laboratory

BigPanDA TIM Meeting

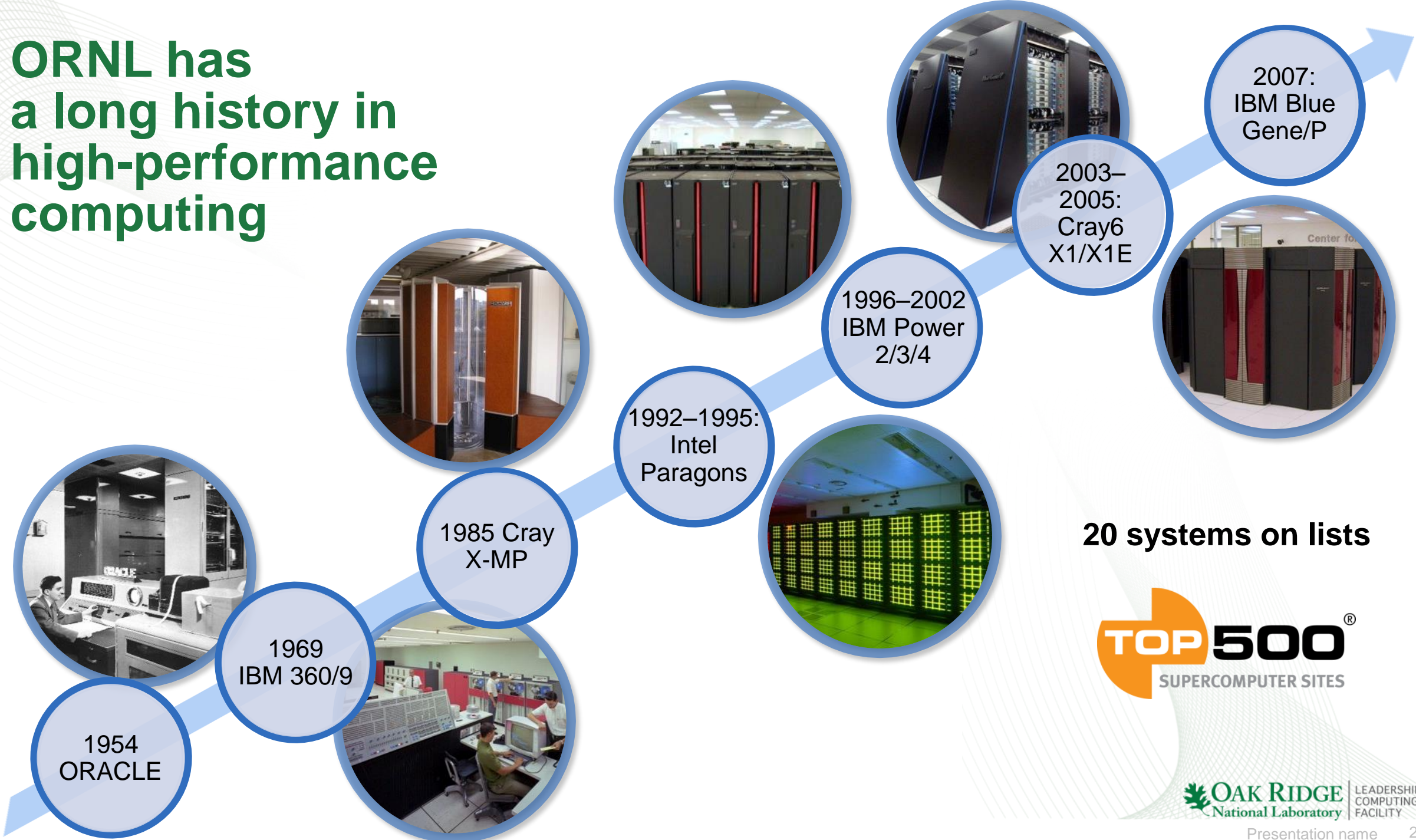
30 March 2017

Oak Ridge

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



# ORNL has a long history in high-performance computing



1954  
ORACLE



1969  
IBM 360/9



1985 Cray  
X-MP



1992-1995:  
Intel  
Paragons



1996-2002  
IBM Power  
2/3/4



2003-  
2005:  
Cray6  
X1/X1E



2007:  
IBM Blue  
Gene/P

20 systems on lists



# Oak Ridge Leadership Computing Facility (OLCF) is one of the world's most powerful computing facilities



## Titan

Peak performance	27 PF/s
Memory	710 TB
Disk bandwidth	240 GB/s
Square feet	5,000
Power	8.8 MW

## Data storage

- Spider file system
  - 40 PB capacity
  - >1 TB/s bandwidth
- HPSS archive
  - 240 PB capacity
  - 6 tape libraries

## Gaea

Peak performance	1.1 PF/s
Memory	240 TB
Disk bandwidth	104 GB/s
Square feet	1,600
Power	2.2 MW

## Data analytics/visualization

- LENS cluster
- Ewok cluster
- EVEREST visualization facility
- uRiKA data appliance

## Beacon

Peak performance	210 TF/s
Memory	12 TB
Disk bandwidth	56 GB/s

## Networks

- ESnet, 100 Gbps
- Internet2, 100 Gbps
- Private dark fibre

## Eos

Peak performance	240.9 TF/s
Memory	47 TB
Disk bandwidth	30 GB/s

# CADES Zones and Scope



HEALTH DATA SCIENCES INSTITUTE  
OAK RIDGE NATIONAL LABORATORY



CLIMATE CHANGE  
SCIENCE INSTITUTE  
OAK RIDGE NATIONAL LABORATORY



BESC  
BioEnergy Science Center

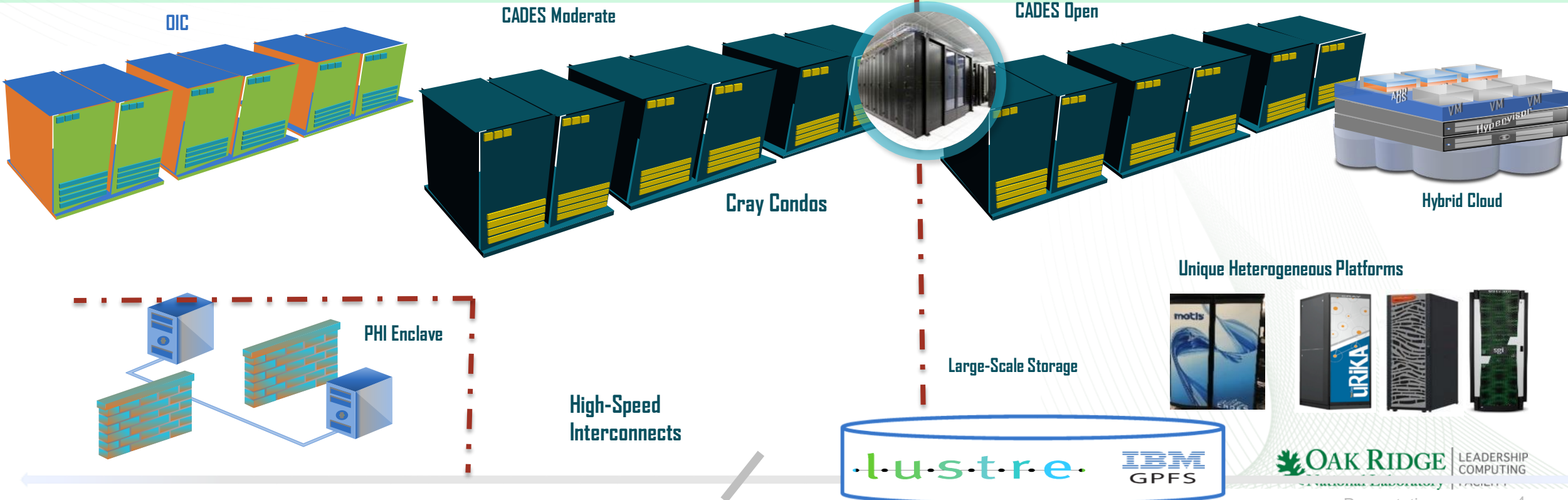


.. and several ORNL projects on OIC

.. and several other smaller projects.

- ~5000 Cores of Integrated Condos on Infiniband
- ~10,000 OIC Cores
- Attested PHI Enclave
- Integrated with UCAMS and XCAMS

- ~6000 Cores of Integrated Condos on Infiniband
- ~5000 Cores of Hybrid, Expandable Cloud
- SGI UV, Urika-GD/XA: GX
- 5PB+ High-Speed Storage
- ~3000 Cores of XK7



# Origin of Leadership Computing Facilities

## 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

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,

### SECTION 1. SHORT TITLE.

This Act may be cited as the "Department of Energy High-End Computing Revitalization Act of 2004".

### 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.

### 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;

Nov. 30, 2004  
[H.R. 4516]

Department of Energy High-End Computing Revitalization Act of 2004.  
15 USC 5501 note.  
15 USC 5541.

15 USC 5542.

# DOE Office of Science National User Facilities



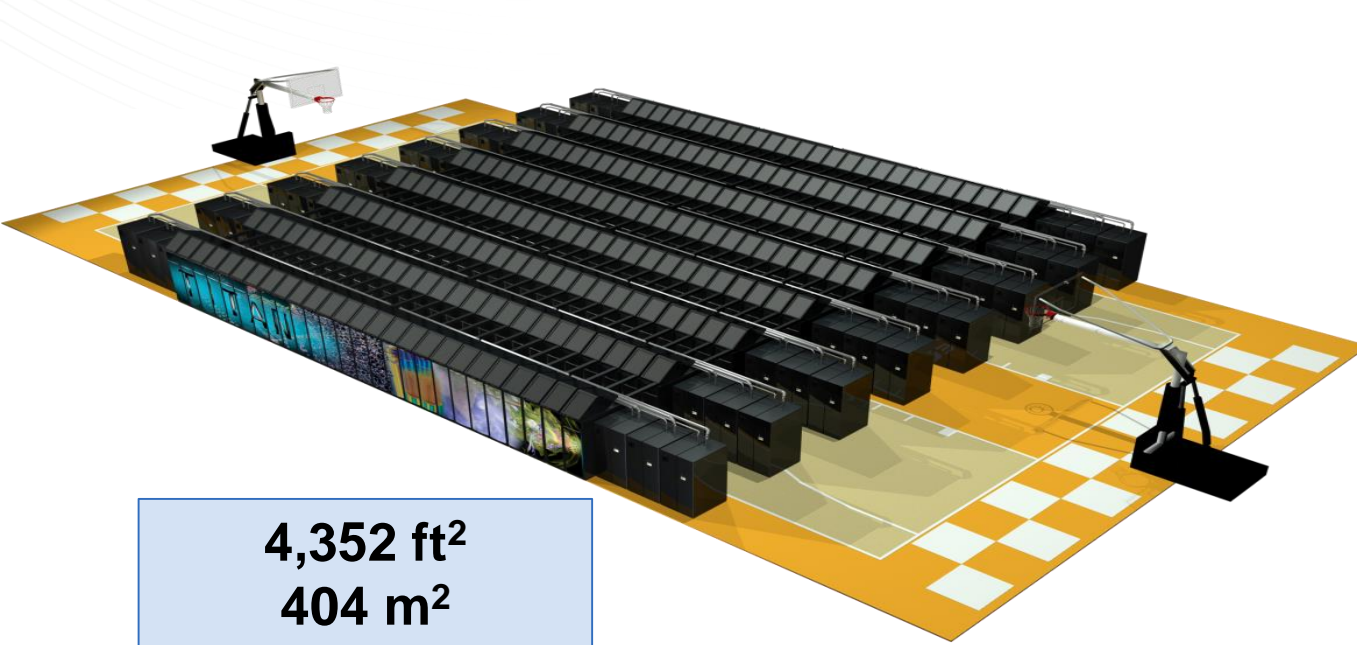
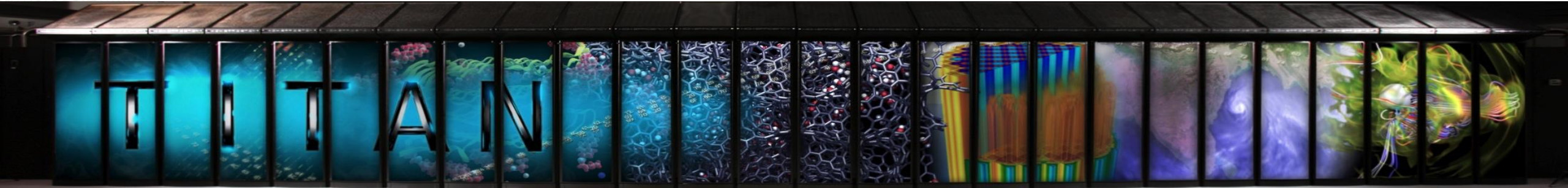
28 world-leading facilities serving over 33,000 researchers annually

- supercomputers,
  - high intensity x-ray, neutron, and electron sources,
  - nanoscience facilities,
  - genomic sequencing facilities,
  - particle accelerators,
  - fusion/plasma physics facilities, and
  - atmospheric monitoring capabilities.
- 
- **Open access; allocation determined through peer review of proposals**
  - **Free for non-proprietary work published in the open literature**
  - **Full cost recovery for proprietary work**

<http://science.energy.gov/user-facilities/user-facilities-at-a-glance/>

# ORNL's "Titan" Hybrid System: Nation's Most Powerful Computer for Open Science

#3 **TOP 500**  
SUPERCOMPUTER SITES



4,352 ft<sup>2</sup>  
404 m<sup>2</sup>

## 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

# Three primary user programs for access to LCF

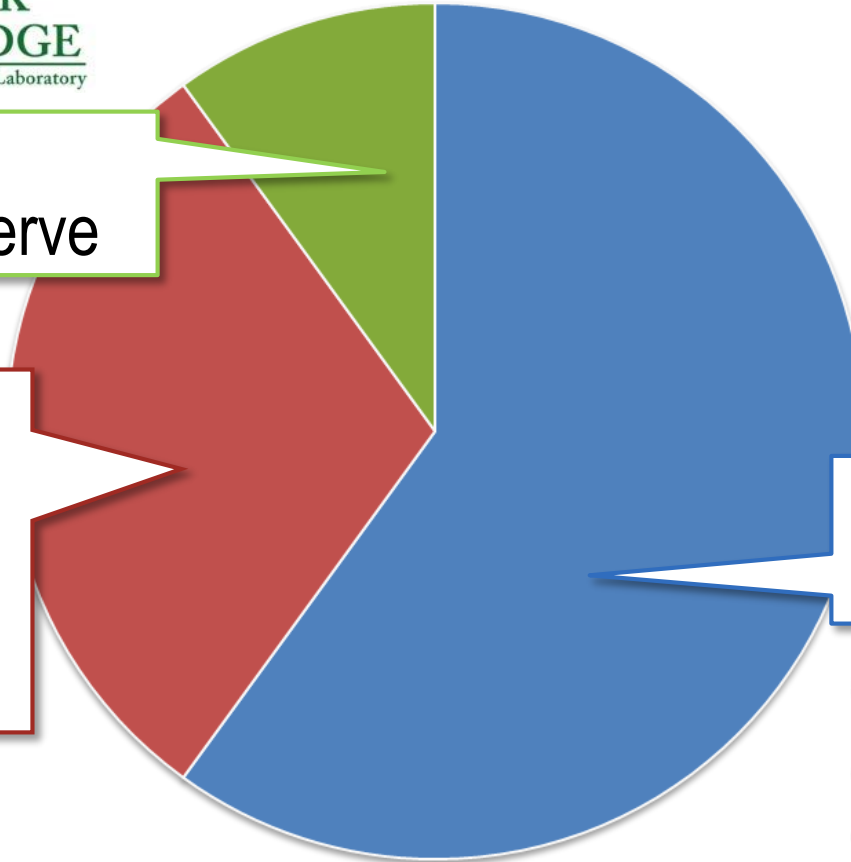
## *Distribution of allocable hours*



10% Director's  
Discretionary Reserve

**30% ALCC**

ASCR Leadership  
Computing  
Challenge



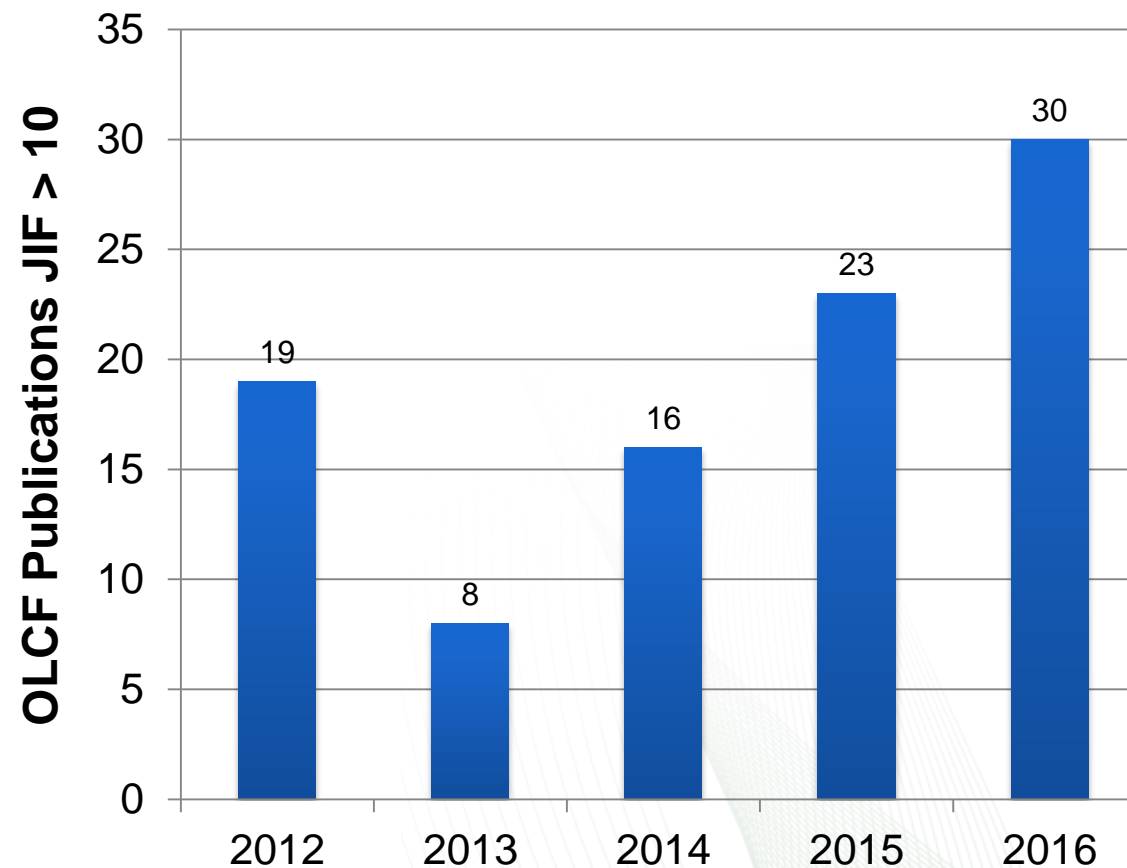
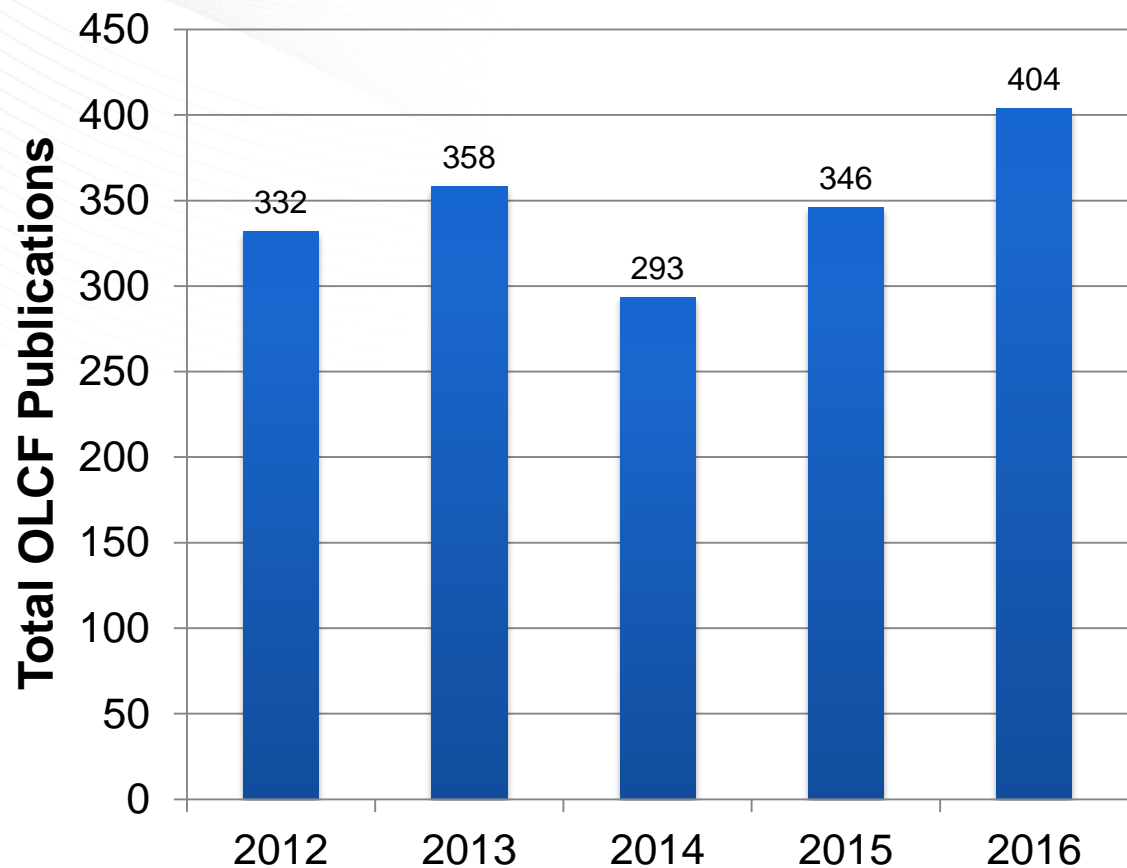
**60% INCITE**



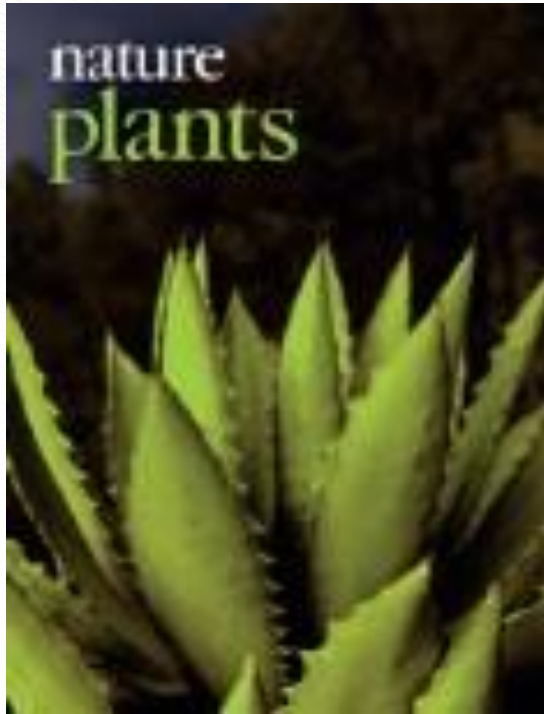
# OLCF allocation programs: Selecting applications of national importance

	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 (2015 example)	30 projects per year	13M - 170M core-hours/yr. (2015 avg-75M)	24 projects per year	5M – 250M core-hours/yr. (2015 avg-49M)	~120 of projects	10K – 30M core-hours (2015 avg-3.1M)
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review		Peer-Review & Alignment with Goals	
Managed by	INCITE management committee (ALCF & OLCF)		DOE Office of Science		OLCF management	
Availability	Open to all scientific researchers and organizations including industry					

# OLCF Publication Productivity is Strong

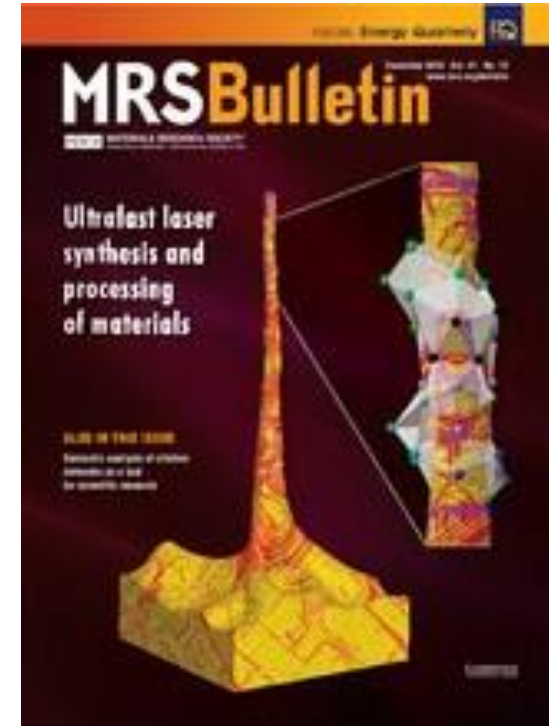


# OLCF Projects Capture Multiple Journal Covers



A multi-disciplinary team is using Titan to understand the most water-efficient form of photosynthesis (called CAM) and how it may be genetically engineered into feed stock, food, and bioenergy crops. The work made the cover of the December 12, 2016 issue of *Nature Plants*.

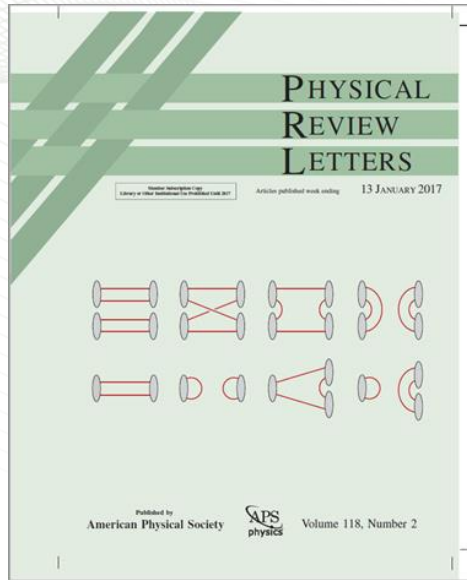
<http://www.nature.com/articles/nplants2016178>



Researchers from the University of Virginia are using Titan to understand laser interactions with metallic surfaces at a molecular level. The team has been doing multi-billion-particle simulations, and has increased its time to solution by sevenfold. The work was on the December, 2016 cover of *MRS Bulletin*.

<https://www.cambridge.org/core/journals/mrs-bulletin/article/div-classtitlefundamentals-of-ultrafast-lasermaterial-interactiondiv/3531E1E15FD75A2BC189A21B911431E0>

# OLCF Projects Capture Multiple Journal Covers



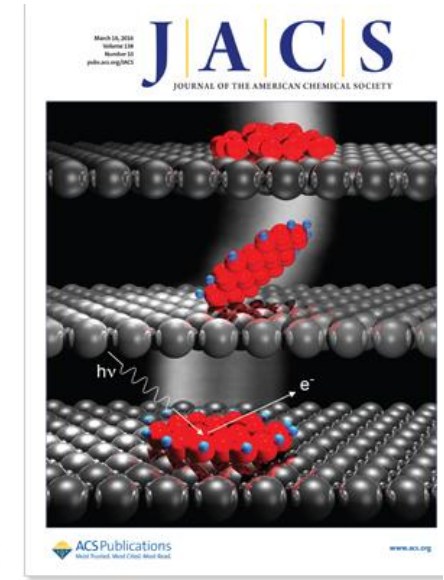
A multi-institution team led by Jefferson Lab's Robert Edwards used OLCF resources to support research into exotic states of matter. The work supports efforts that are part of Jefferson Lab's GlueX experiment. The team earned the January 9 cover of *Physical Review Letters* for its simulation of the origin of the “sigma” particle—a mystery for 50 years.

<http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.118.022002>



A research team led by Virginia Tech's James McClure uses Titan to study subsurface flows to improve carbon sequestration methods and oil and gas recovery efforts. The team's finding that “disconnected” oil reserves that are not connected to a larger reservoir still play an active role in contributing to subsurface flows. The team's work earned the best paper at the Society of Core Analysts meeting and was given the cover of *Petrophysics*.

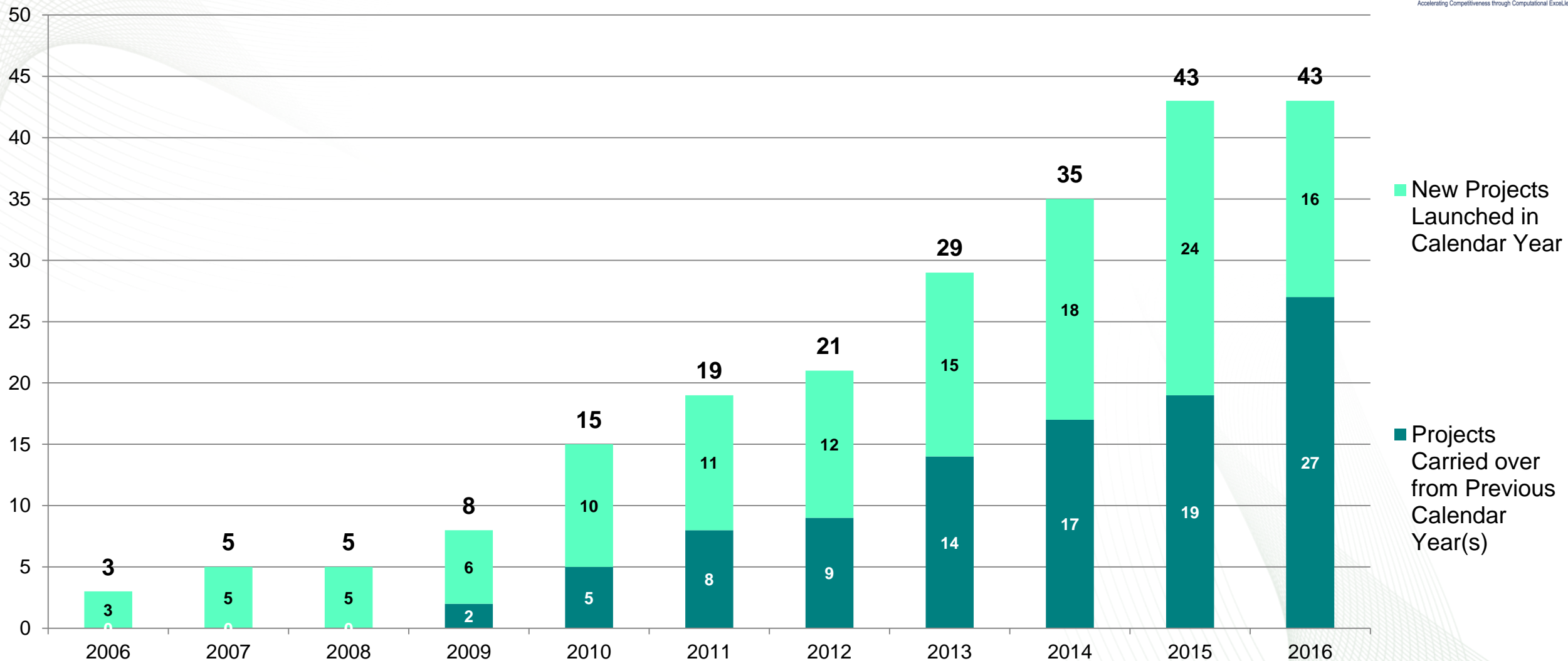
<https://www.onepetro.org/journal-paper/SPWLA-2017-v58n1a1>



Researchers led by University College London researcher Dario Alfé used supercomputing simulations to gain a deeper understanding of large molecule adsorption at the atomic level. The team was featured on the March 16, 2016 edition of the *Journal of the American Chemical Society* due to their new insights into molecular breakup.

<http://pubs.acs.org/doi/abs/10.1021/jacs.5b12504>

# Number of OLCF Industry Projects by Calendar Year





**Diversity in numbers**  
Over 150 projects in a wide range  
of domains

## User base

- ~1000 users / year
- Mixture of developers and turnkey
- Have previous HPC experience
- Graduate students and postdocs

# Questions?

[wellsjc@ornl.gov](mailto:wellsjc@ornl.gov)

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