Accelerating computational science and engineering with leadership computing

20 Years of Excellence in Computational Science

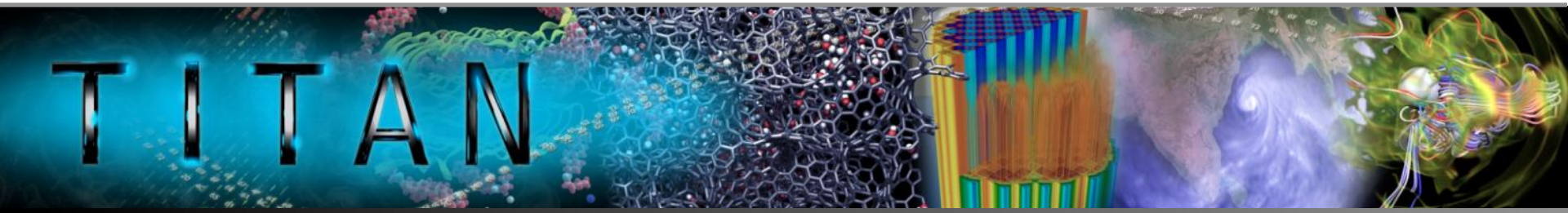
OLCF

Oak Ridge Leadership Computing Facility

1992–2012

Jack C. Wells
Director of Science
Oak Ridge Leadership Computing Facility

NVIDIA Theatre @ SC13



Big Problems Require Big Solutions

Climate Change

Energy

Healthcare

Competitiveness

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).

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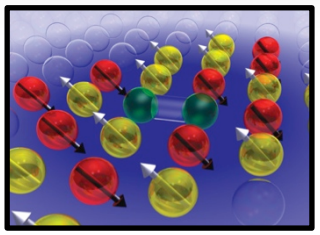
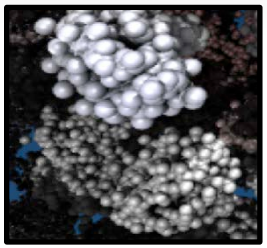
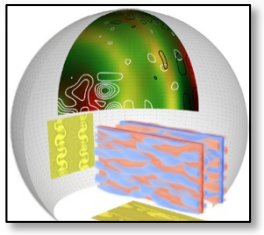
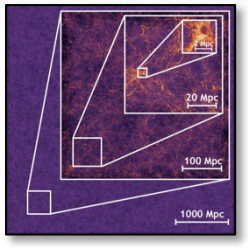
Argonne NATIONAL LABORATORY

#2 TOP500 SUPERCOMPUTER SITES

Titan System (Cray XK7)			
Peak Performance	27.1 PF 18,688 compute nodes	24.5 PF GPU	2.6 PF CPU
LINPACK Performance	17.59 PF		
Power	8.2 MW		
System Memory	710 TB total memory		
Interconnect	Gemini High Speed Interconnect	3D Torus	
Storage	Luster Filesystem	32 PB	
Archive	High-Performance Storage System (HPSS)	29 PB	
I/O Nodes	512 Service and I/O nodes		

High-impact science at OLCF: Four of Six SC13 Gordon Bell Finalists Used Titan

Peter Staar ETH Zurich	Massimo Bernaschi ICNR-IAC Rome	Michael Bussmann HZDR - Dresden	Salman Habib Argonne
High-Temperature Superconductivity	**Biofluidic Systems**	**Plasma Physics**	**Cosmology**
Taking a Quantum Leap in Time to Solution for Simulations of High-T_C Superconductors	20 Petaflops Simulation of Protein Suspensions in Crowding Conditions	Radiative Signatures of the Relativistic Kelvin-Helmholtz Instability	HACC: Extreme Scaling and Performance Across Diverse Architectures
Titan (15.4 PF)	Titan (20 PF)	Titan (7.2 PF)	Sequoia (13.9 PF), Titan
			

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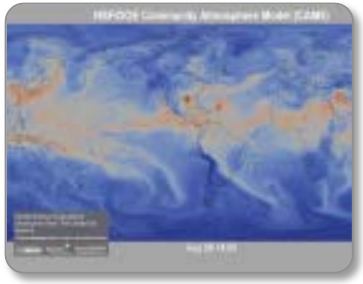
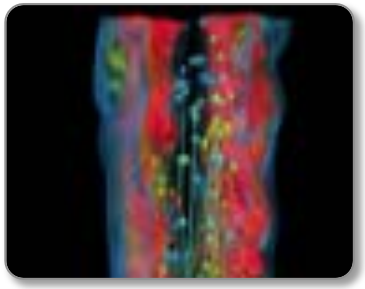
Science challenges for LCF in next decade



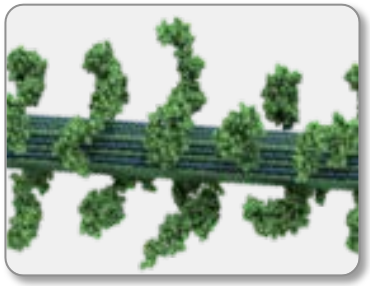
Climate Change Science
Understand the dynamic ecological and chemical evolution of the climate system with uncertainty quantification of impacts.

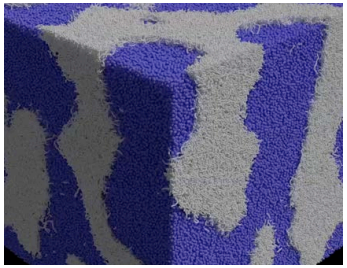
Combustion Science
Increase efficiency by 25%-50% and lower emissions from internal combustion engines using advanced fuels and low-temperature combustion.



Fusion Energy
Develop predictive understanding of plasma properties, dynamics, and interactions with surrounding materials.

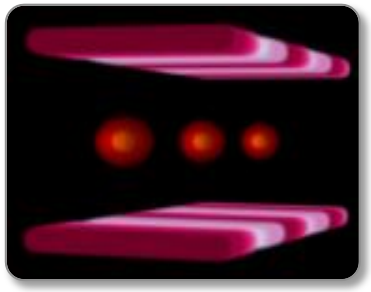
Biomass to Biofuels
Enhance the understanding and production of biofuels for transportation and other bio-products from biomass.





Solar Energy
Improve photovoltaic efficiency and lower cost for organic and inorganic materials.

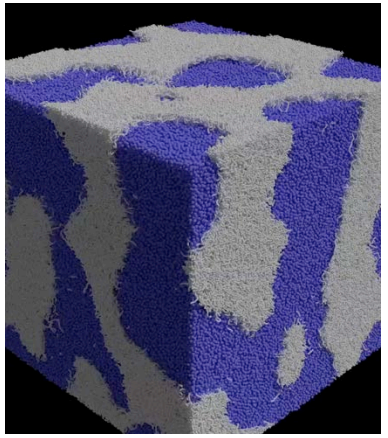
Optimized Accelerator Designs
Optimize designs as the next generations of accelerators . Detailed models are needed to provide efficient designs of new light sources.



Solar energy

Key science challenges: Improve photovoltaic efficiency and lower cost for organic and inorganic materials.

A photovoltaic material poses difficult challenges in the prediction of morphology, excited state phenomena, transport, and materials aging.

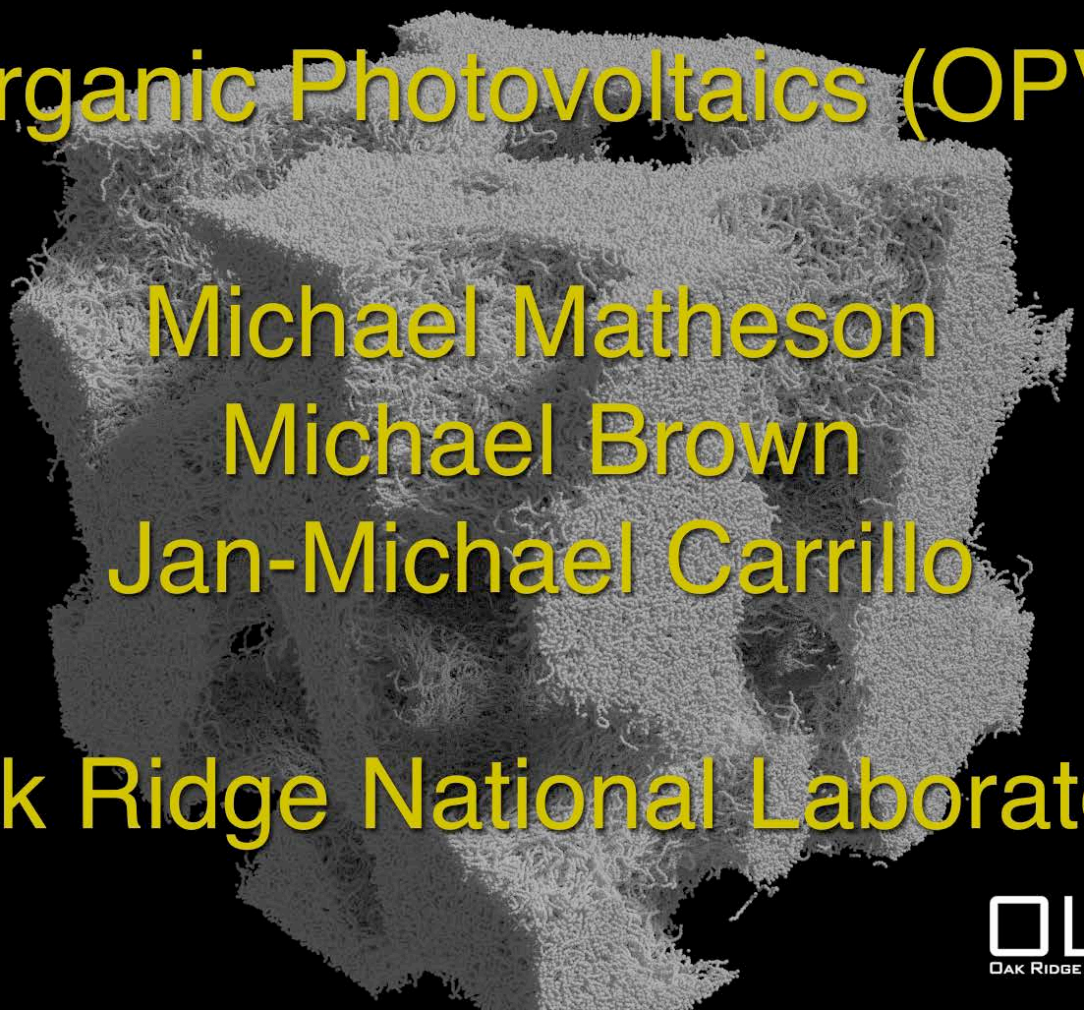


Corse-grained MD simulation of phase-separation of a 1:1 weight ratio P3HT/PCBM mixture into donor (white) and acceptor (blue) domains.

Science enabled by LCF Capabilities

2013-2016	2016-2020
• Understand growth, interface structure, and stability of heterogeneous polymer blends necessary for efficient solar conversion. • Simulations of structure, carrier transport, and defect states in nanomaterials. • Describe excited state phenomena in homogeneous systems.	• Enable computational screening of materials for desired excited-state and charge transport properties. • Systems-level, multiphysics simulations of practical photovoltaic devices are enabled. • Uncertainty quantification enabled for critical integrated materials properties.

Organic Photovoltaics (OPV)



Michael Matheson
Michael Brown
Jan-Michael Carrillo

Oak Ridge National Laboratory

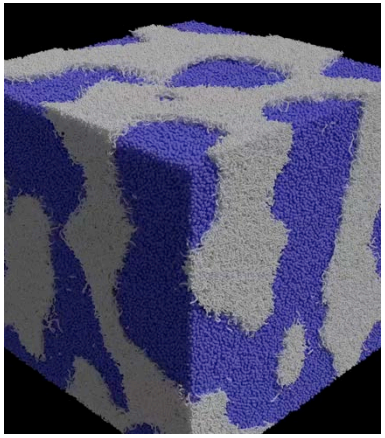
OLCF
Oak Ridge Leadership Computing Facility

Towards Rational Design of Efficient Organic Photovoltaic Materials

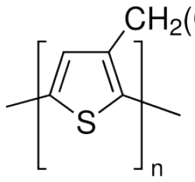
LAMMPS Early Science Project
Jan-Michael Carrillo, ORNL
Mike Brown, ORNL

Science Objectives and Impact

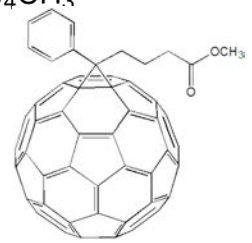
- Organic photovoltaic (OPV) solar cells are promising renewable energy sources:
  - Low costs, high-flexibility, and light weight
- Bulk-heterojunction (BHJ) active layer morphology and domain size is critical for improving performance



P3HT (electron donor)



PCBM (electron acceptor)



Corse-grained MD simulation of phase-separation of a 1:1 weight ratio P3HT/PCBM mixture into donor (white) and acceptor (blue) domains.

Titan Simulation: LAMMPS

- Portability: Builds with CUDA or OpenCL
- Speedups on Titan (GPU+CPU vs. CPU: 2X to 15x (mixed precision) depending upon model and simulation
  - Speedup of 2.5-3x for OPV simulation used here

Preliminary Science Results

- Titan simulations are 27x larger and 10x longer
  - Converged P3HT:PCBM separation in 400ns CGMD time
- Prediction: Increasing polymer chain length will decrease the size of the electron donor domains
- Prediction: PCBM (fullerene) loading parameter results in an increasing, then decreasing impact on P3HT domain size

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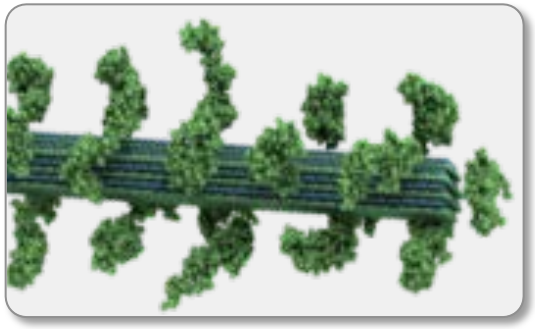
Biomass to biofuels

Key science challenges: Enhance the understanding and production of biofules from biomass for transportation and other bio-products.
The main challenge to overcome is the recalcitrance of biomass (cellulosic materials) to hydrolysis.



Lignin interacting with crystalline cellulose.

Science enabled by increasing LCF Capabilities

2013-2016	2016-2020
• Atomic-detail dynamical models of biomass systems of several million atoms, permitting detailed analysis of interactions	• Understand the dynamics of enzymatic reactions on biomass by simulating interactions between microbial systems and cellulosic biomass
• Simulations of pretreatment effects on multi-component biomass systems to understand the bottlenecks in bioconversion	• Design superior enzymes for conversion of biomass

Cellulosic Ethanol: Simulation of Multicomponent Biomass System

Jeremy Smith
INCITE 2013

Oak Ridge National Laboratory

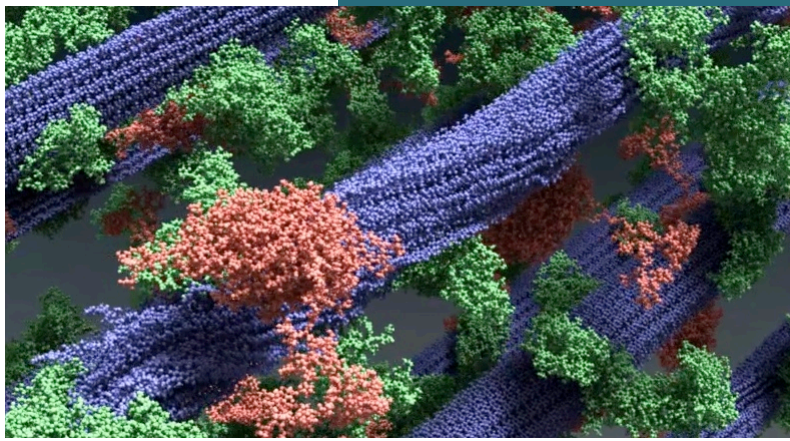
Boosting Bioenergy and Overcoming Recalcitrance

Molecular Dynamics Simulations

INCITE Program
Jeremy Smith
Oak Ridge National Laboratory
23 M Titan core hours

Science Objectives and Impact

- Optimize biomass pretreatment process by understanding lignin-cellulose interactions on a molecular level
- Overcome biomass recalcitrance caused by lignin and the tightly ordered structure of cellulose
- Improve efficiency of the biofuel production process and make ethanol less costly



Interaction between cellulose fibril (blue) and lignin (pink and green) molecules.
Vizualization by M. Matheson (ORNL)

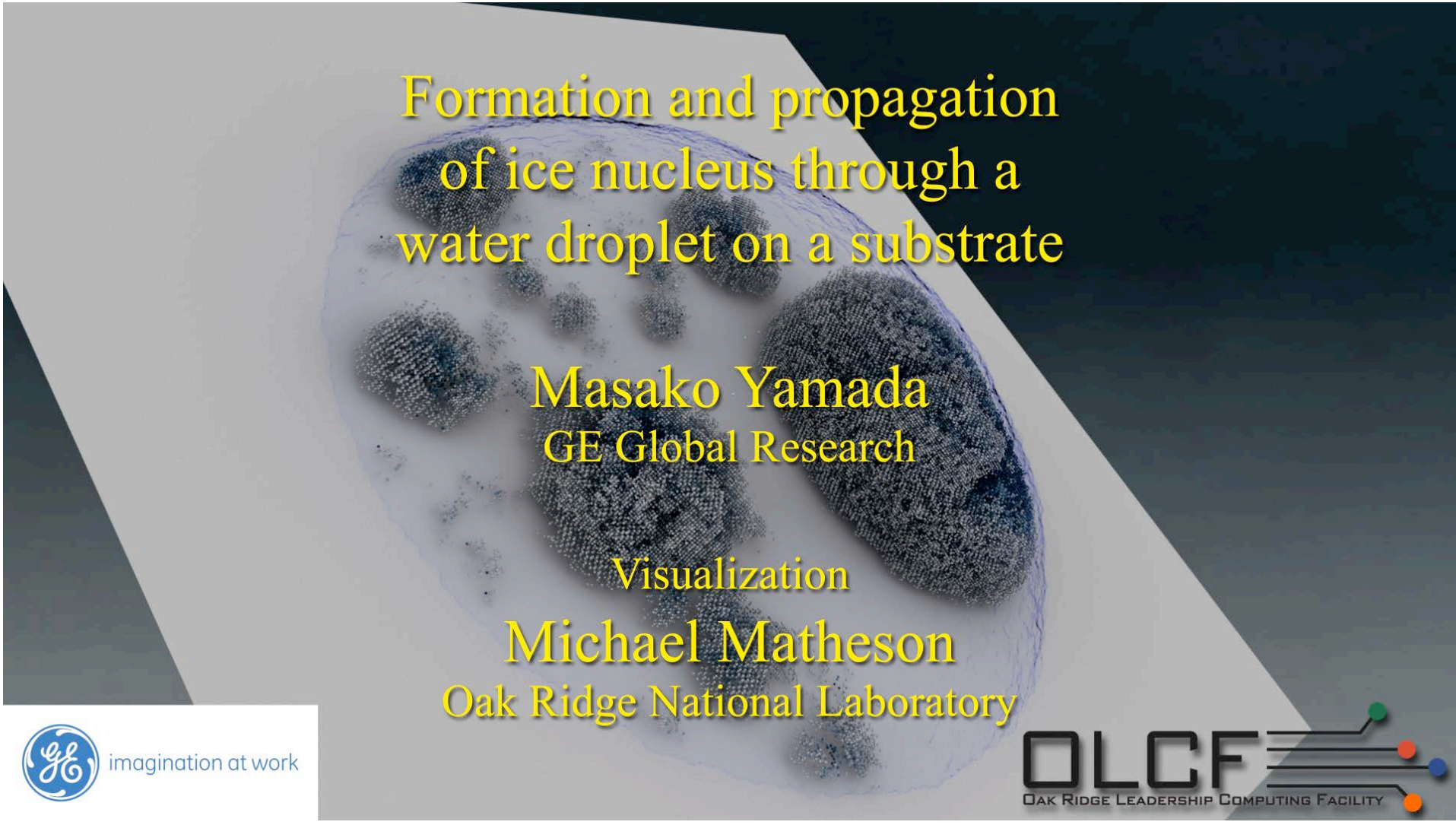
Application Performance

- **2012:** Used GROMACS on Jaguar to monitor interactions of 3 million atoms that included crystalline and non-crystalline cellulose, lignin, and water
- **2013:** Now run accelerated GROMACS that can take advantage of Titan's GPUs, making the application 10 times bigger and much longer. Current simulations monitor 30 million atoms.

Science Results

Published paper in *Biomacromolecules* in August 2013

- Discovered amorphous cellulose is easier to break down because it associates less with lignin
- Phenomenon is not a result of direct interaction between lignin and cellulose, but is a water-mediated effect


Formation and propagation
of ice nucleus through a
water droplet on a substrate
Masako Yamada
GE Global Research
Visualization
Michael Matheson
Oak Ridge National Laboratory
imagination at work
OLCF
Oak Ridge Leadership Computing Facility

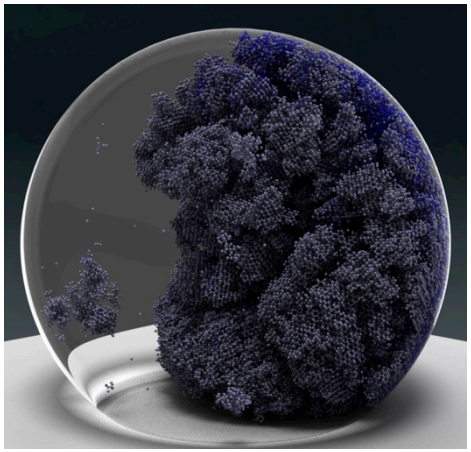
Non-Icing Surfaces for Cold Climate Wind Turbines

Molecular Dynamics Simulations

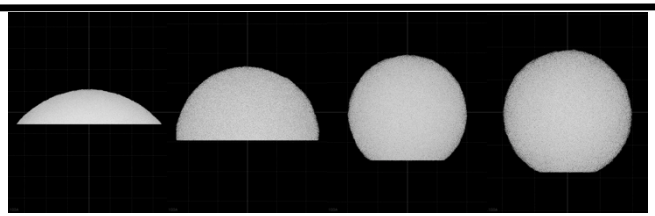
ALCC Program
Masako Yamada
GE Global Research
40 M Titan core hours

Science Objectives and Impact

- Understand microscopic mechanism of water droplets freezing on surfaces
- Determine 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 Achievements

- 5X speed-up from GPU acceleration
- Achieved factor 40X speed-up from new interaction potential for water

Science Results

Replicated GE's experimental results:

- Hydrophobic surfaces delay the onset of nucleation
- The delay is less pronounced at lower temperatures

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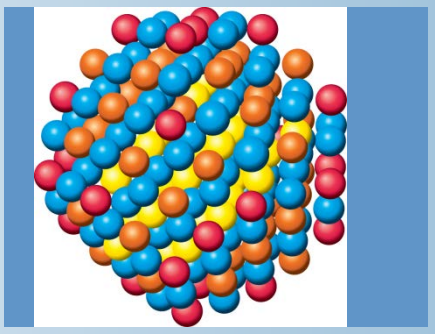
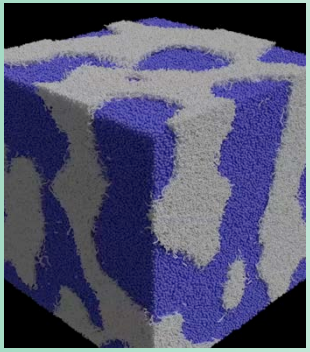
Center for Accelerated Application Readiness (CAAR)

- Focused effort to prepare applications for accelerated architectures
- Goals:
  - Work with code teams to develop and implement strategies for exposing hierarchical parallelism for our users applications
  - Maintain code portability across modern architectures
  - Learn from and share our results
- Selected six applications from different science domains and algorithmic motifs
- Application Teams
  - OLCF application lead
  - Cray engineer
  - NVIDIA developer
  - Others: local tool & library developers, other computational scientists
- Single early science problem targeted for each app
- Explore multiple approached for each app
  - Determine maximum acceleration
  - Determine reproducible path for other applications

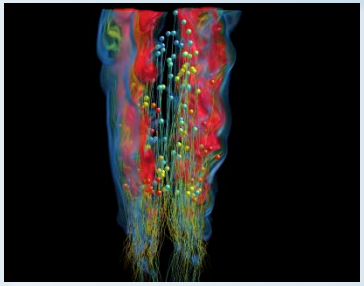
Early Science Challenges for Titan

WL-LSMS
Illuminating the role of material disorder, statistics, and fluctuations in nanoscale materials and systems.





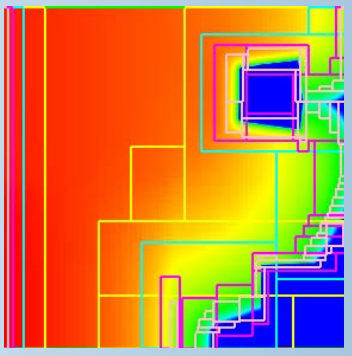
LAMMPS
A molecular dynamics simulation of organic polymers for applications in organic photovoltaic heterojunctions , de-wetting phenomena and biosensor applications

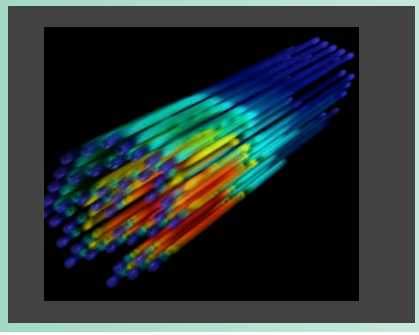


S3D
Understanding turbulent combustion through direct numerical simulation with complex chemistry.
.

CAM-SE
Answering questions about specific climate change adaptation and mitigation scenarios; realistically represent features like precipitation patterns / statistics and tropical storms.

NRDF
Radiation transport – important in astrophysics, laser fusion, combustion, atmospheric dynamics, and medical imaging – computed on AMR grids.





Denovo
Discrete ordinates radiation transport calculations that can be used in a variety of nuclear energy and technology applications.

Effectiveness of GPU Acceleration

	Application	Domain	Cray XK7 vs. Cray XE6 Performance Ratio*
CAAR	LAMMPS	Molecular dynamics	7.4
CAAR	S3D	Turbulent combustion	2.2
CAAR	Denovo	3D neutron transport for nuclear reactors	3.8
CAAR	WL-LSMS	Statistical mechanics of magnetic materials	3.8
Community	AWP-ODC	Seismology	2.1
Community	DCA++	Condensed Matter Physics	4.4
Community	QMCPACK	Electronic structure	2.0
Community	RMG (DFT – real-space, multigrid)	Electronic Structure	2.0
Community	XGC1	Plasma Physics for Fusion Energy R&D	1.8

Titan: Cray XK7 (Kepler GPU plus AMD 16-core Opteron CPU)
Cray XE6: (2x AMD 16-core Opteron CPUs)
*Performance depends strongly on specific problem size chosen

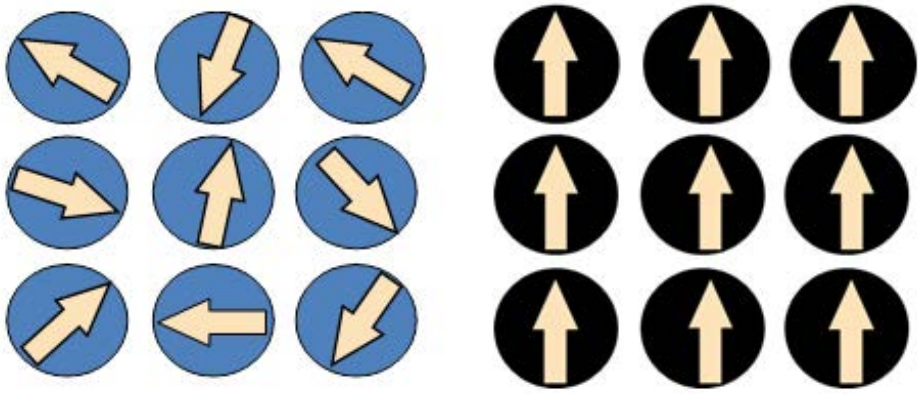
Magnetic Materials

Simulating nickel atoms pushes double-digit petaflops

WL-LSMS
Marcus Eisenbach,
ORNL

Science Objectives and Impact

- Enhance the understanding of microscopic behavior of magnetic materials
- Enable the simulation of new magnetic materials
  - Better, cheaper, more abundant materials
- Model development on Titan will enable investigation on smaller computers



Researchers using Titan are studying the behavior of magnetic systems by simulating nickel atoms as they reach their Curie temperature—the threshold between order (right) and disorder (left).

Titan Simulation: WL-LSMS

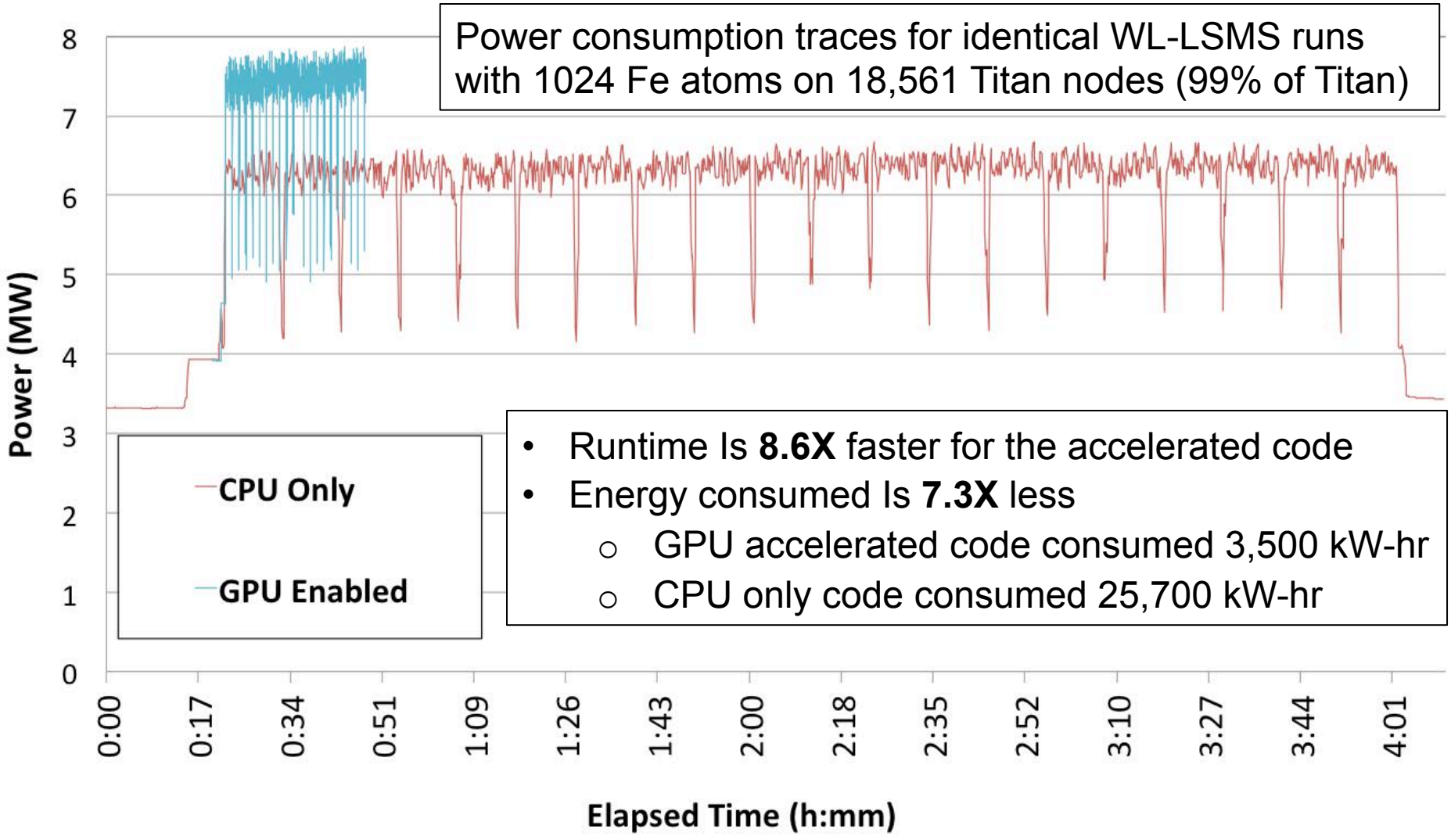
- More than an 8-factor speedup on Titan compared to Jaguar, Cray XT-5
  - From 1.84 PF to 14.5 PF
- Wang-Landau allows for calculations at realistic temperatures

Preliminary Science Results

- Titan necessary to calculate nickel's Curie temperature, a more complex calculation than iron
- Calculated 50 percent larger phase space
- Four times faster on Titan than on comparable CPU-only system, (i.e., Cray XE6).

Application Power Efficiency of the Cray XK7

WL-LSMS for CPU-only and Accelerated Computing



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All Codes Will Need Rework at Scale!

- **Up to 1-2 person-years required to port each code from Jaguar to Titan**
  - Takes work, but an unavoidable step **required for exascale regardless of the type of processors.** It comes from the required level of **parallelism on the node**
  - Also **pays off for other systems**—the ported codes often run significantly faster CPU-only (Denovo 2X, CAM-SE >1.7X)
- We estimate possibly **70-80% of developer time is spent in code restructuring**, regardless of whether using OpenMP / CUDA / OpenCL / OpenACC / …
- **Each code team must make its own choice of using OpenMP vs. CUDA vs. OpenCL vs. OpenACC**, based on the specific case—may be different conclusion for each code
- **Our users and their sponsors must plan for this work.**

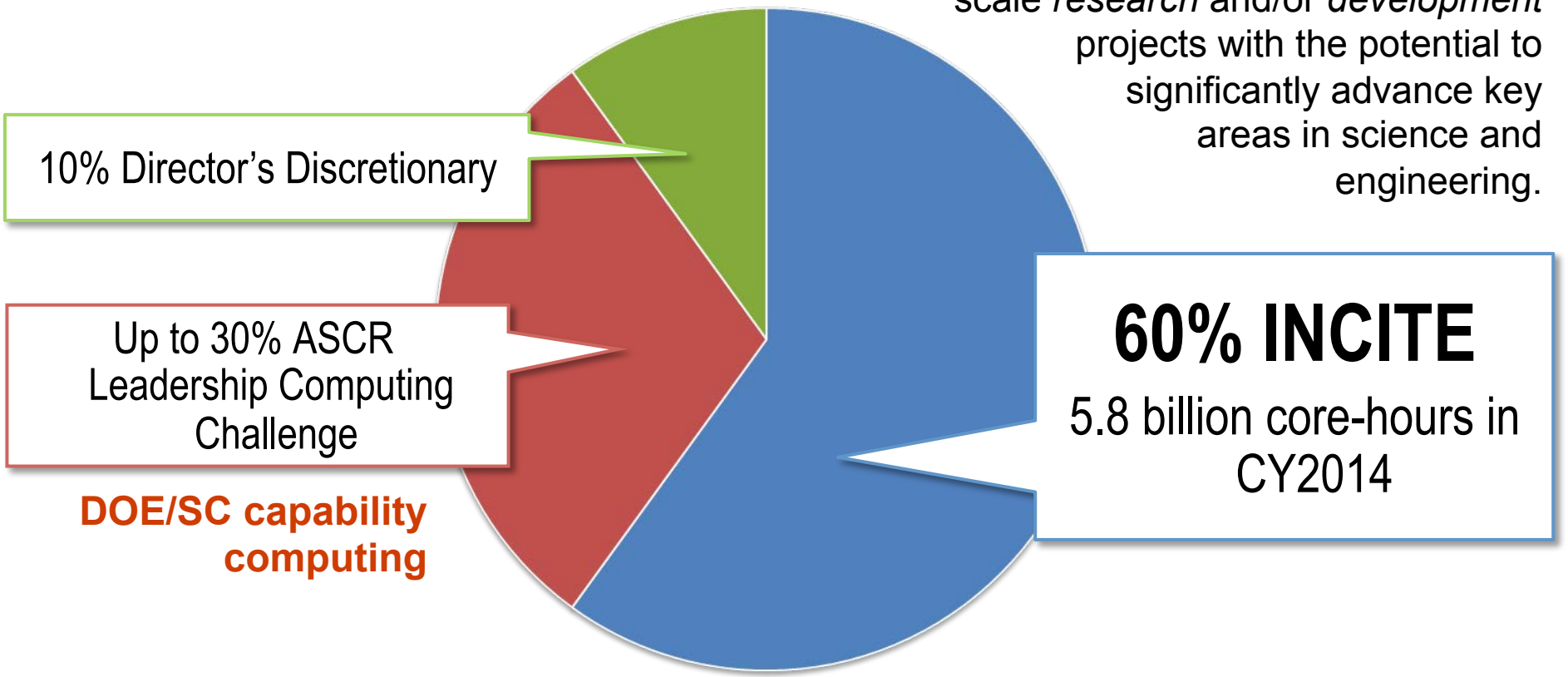
More Lessons Learned

- Science codes are under active development—porting to GPU can be pursuing a "moving target," challenging to manage
- Heterogeneous architectures can make previously infeasible or inefficient models and implementations viable
- More available FLOPS on the node should lead us to think of new science opportunities enabled—e.g., more degrees of freedom per grid cell
- We may need to look to new ideas to get another ~30X thread parallelism that may be needed for exascale—e.g., parallelism in time, uncertainty quantification, design of experiments

Three primary ways for access to LCF
Distribution of allocable hours

Leadership-class computing

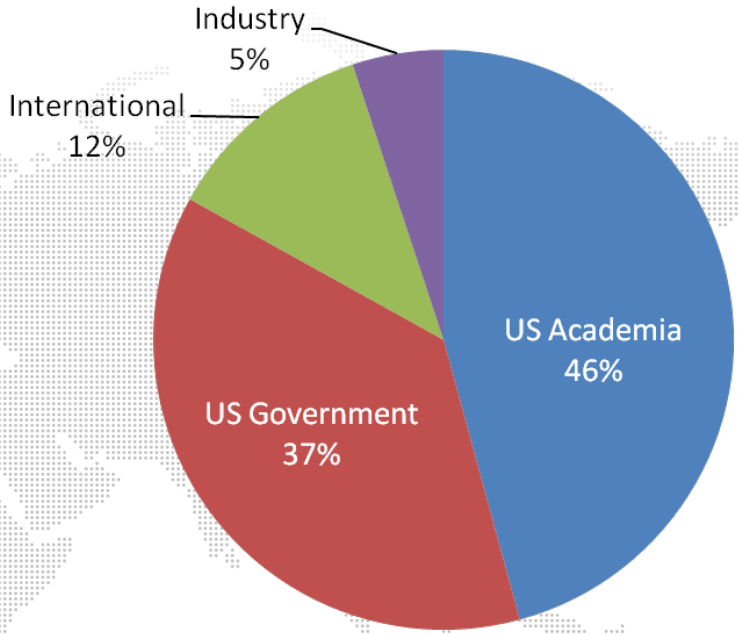
INCITE seeks computationally intensive, large-scale *research* and/or *development* projects with the potential to significantly advance key areas in science and engineering.



2014 INCITE award statistics

- Request for Information helped attract new projects
- Call closed June 28th, 2013
- Total requests **~14 billion core-hours**
- Awards of 5.8 billion core-hours for CY 2014
- **59 projects awarded of which 21 are renewals**

PIs by Affiliation (Awards)



Acceptance rates

- *36% of nonrenewal submittals*
- *91% of renewals*

Contact information
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MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Conclusions

- Leadership computing is for the critically important problems that need the most powerful compute and data infrastructure
- Accelerated, hybrid-multicore computing solutions are performing well on real, complex scientific applications.
  - But you must work to expose the parallelism in your codes.
  - This refactoring of codes is largely common to all massively parallel architectures
- OLCF resources are available to industry, academia, and labs, through open, peer-reviewed allocation mechanisms.

Acknowledgements

OLCF-3 CAAR Team:

- Bronson Messer, Wayne Joubert, Mike Brown, Matt Norman, Markus Eisenbach, Ramanan Sankaran

OLCF-3 Vendor Partners: Cray, AMD, NVIDIA, CAPS, Allinea

OLCF Users: Jeremy Smith(UT/ORNL), Masako Yamada (GE)

Mike Matheson (ORNL) for visualizations

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Questions?

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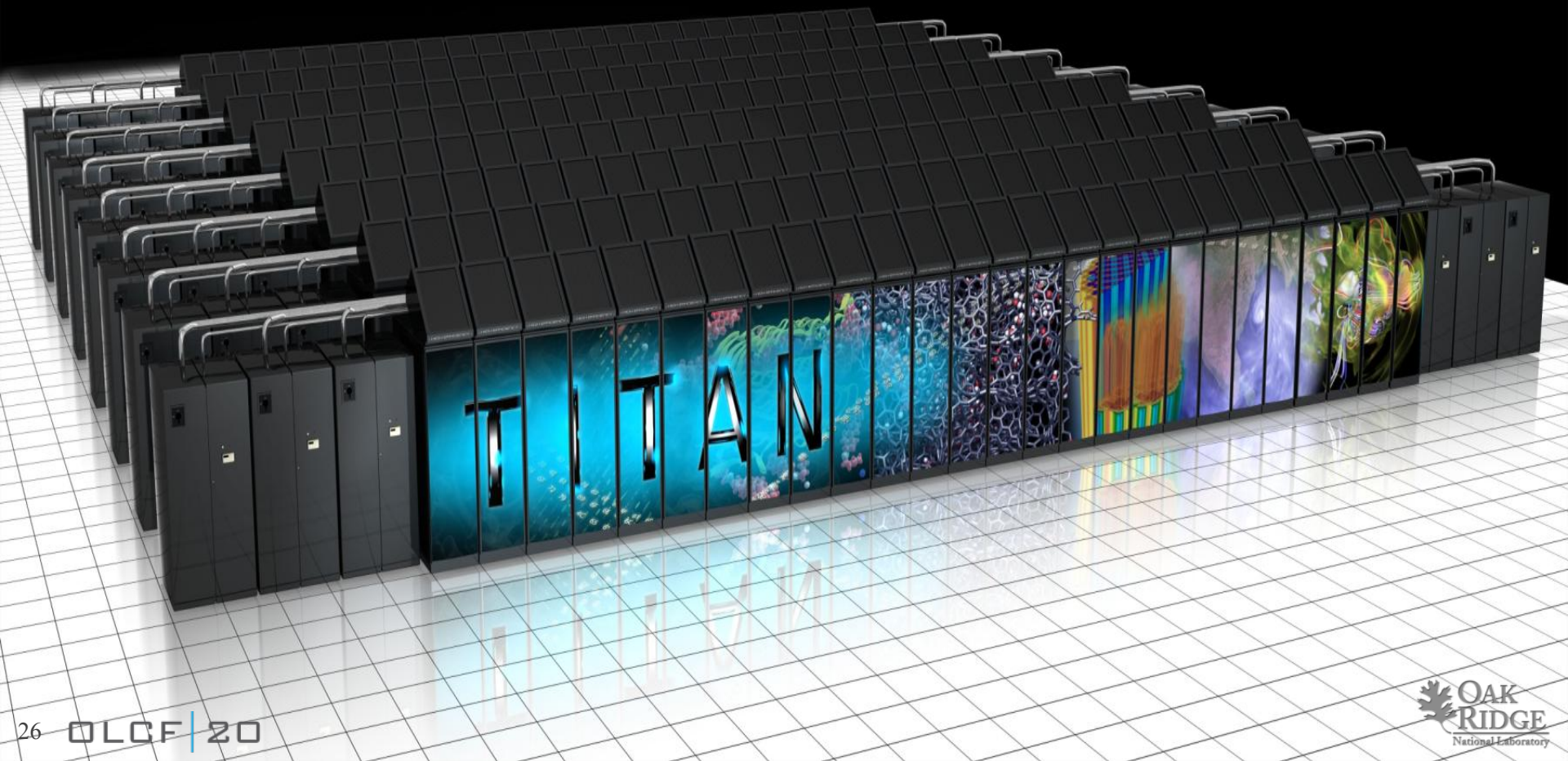
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