# DOE transforms HPC



OAK RIDGE National Laboratory

CADES - The Compute and Data Environment for Science

Breakthrough Science at Every Scale

Computer Science and Mathematics at ORNL

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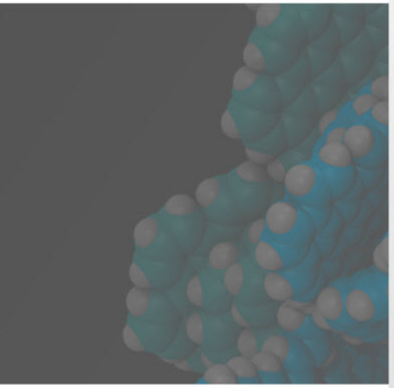
OAK RIDGE National Laboratory



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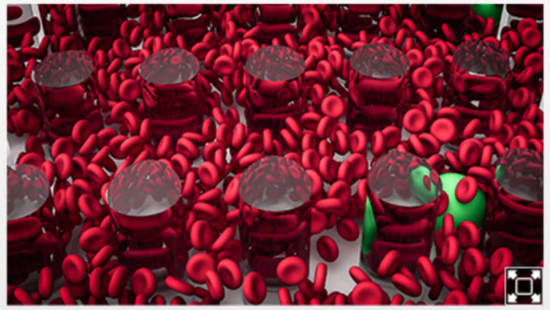
# Breakthrough Science at Every Scale

The Oak Ridge Leadership Computing Facility (OLCF) is one of two DOE leadership computing facilities and was established at Oak Ridge National Laboratory in 2004 with the mission of accelerating scientific discovery and engineering progress. The OLCF achieves this mission by providing world-leading computational performance and an advanced data infrastructure. The OLCF allocates supercomputing resources that substantially exceed those commonly available for research. Instrumental in breakthroughs in biology, chemistry, seismology, engineering, energy, and other fields, OLCF simulations have improved the safety and performance of nuclear power plants, turbomachinery, and aircraft; aided understanding of climate change; accelerated development of new drugs and advanced materials; and guided design of an international fusion reactor. The simulations have explored supernovas, hurricanes, biofuels, neurodegenerative diseases, and clean combustion for power and propulsion. Research challenges remain, and OLCF resources can help.

Approximately 1,200 researchers per year from industry, academia, and government use the OLCF to push the frontiers of their research. Experienced at deploying world-class systems to meet the needs of researchers, the OLCF offers a team of experts including computational scientists that enable broad use and applicability of high-performance computing technologies coupled with data analytics, visualization, storage, and networks at the highest level of capability.



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*The National Laboratory System*

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U.S. DEPARTMENT OF ENERGY

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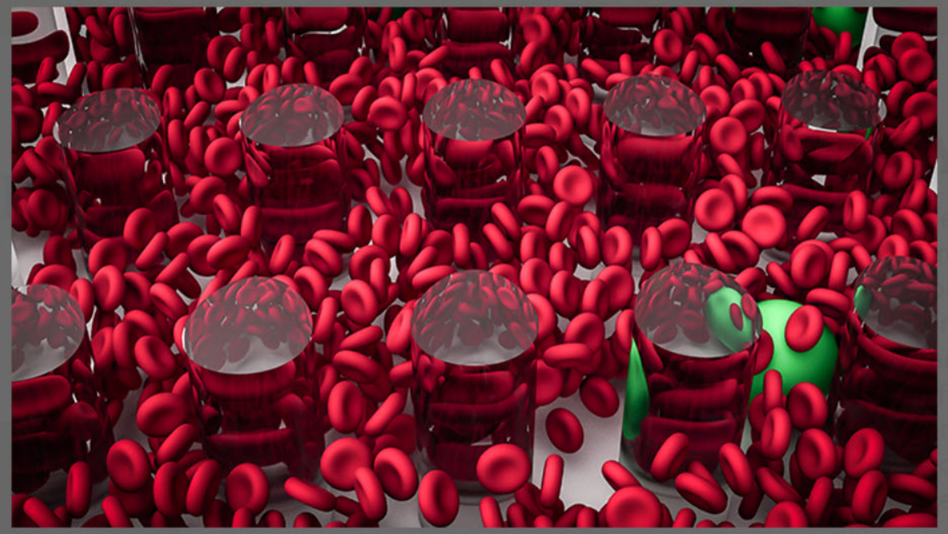

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## Scale

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Funded by the Department of Energy's Office of Advanced Scientific Computing Research.

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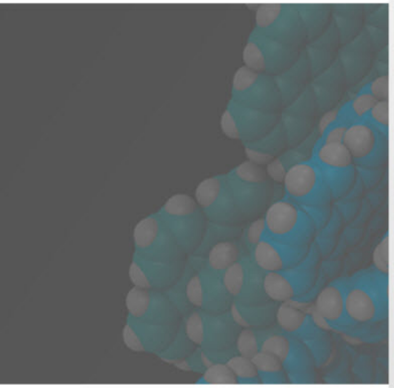

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# Computer Science and Mathematics at ORNL

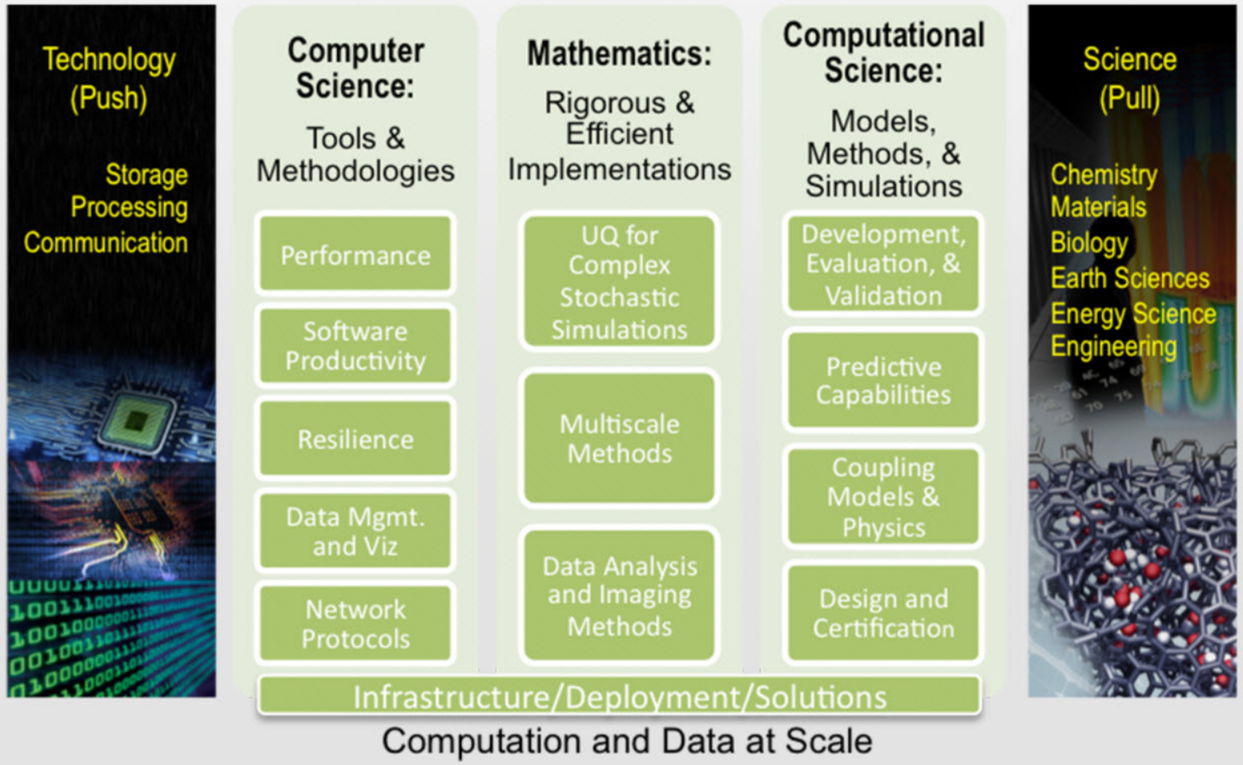
www.csm.ornl.gov

Research programs in the Computer Science and Mathematics Division at ORNL are focused on the computational technologies, methods, and tools needed to address scientific and engineering challenges related to energy. Our goal is to develop the computational infrastructure and ecosystem needed to enable scientific discoveries and predictions with clearly articulated confidence, emphasizing extreme scale systems used for simulations and data analysis.

The organization includes research groups that are engaged in science and engineering applications, applied mathematics, complex systems, and computer science. With this range of expertise, building vertically integrated teams that include computational scientists, mathematicians and computer scientists has become a normal part of our operation. This integration enhances our ability to consider cross-domain improvements. Given the rapid changes in computing technologies, these vertically integrated teams are critical in understanding the impact of new computational technologies on applications and how emerging technologies can be adapted to meet the needs of the applications.

**Computer Science and Mathematics Capabilities**

- Integration of modeling and simulation with experiments and observations
- Emphasis on scientific data, models, and simulations
- Predictive capabilities
- Computation at scale
- Coupled physics
- Emerging platforms
- Vertical Integration



# Computer Science and Mathematics Division

## CSMD

The Computer Science and Mathematics Division (CSMD) is ORNL's premier source of basic and applied research in high-performance computing, applied mathematics, and intelligent systems. Basic and applied research programs are focused on computational sciences, intelligent systems, and information technologies.

Our mission includes working on important national priorities with advanced computing systems, working cooperatively with U.S. Industry to enable efficient, cost-competitive design, and working with universities to enhance science education and scientific awareness. Our researchers are finding new ways to solve problems beyond the reach of most computers and are putting powerful software tools into the hands of students, teachers, government researchers, and industrial scientists.

## News

**Rao Receives Patent**

Nagi Rao received a patent for his work - Failure detection in high-performance clusters and computers using chaotic map computations

This patent relates to failure detection and more particularly to fault detection of computing machines that utilize multiple processor cores and accelerators.

A programmable media includes a processing unit capable of independent operation in a machine that is capable of executing 10.sup.18 floating point operations per second. The processing unit is in communication with a memory element and an interconnect that couples computing nodes. The programmable media includes a logical unit configured to execute arithmetic functions, comparative functions, and/or logical functions. The processing unit is configured to detect computing component failures, memory element failures and/or interconnect failures by executing programming threads that generate one or more chaotic map trajectories. The central processing unit or graphical processing unit is configured to detect a computing component failure, memory element failure and/or an interconnect failure through an automated comparison of signal trajectories generated by the chaotic maps.

**Opportunities for Nonvolatile Memory Systems in Extreme-Scale High Performance Computing (November 2015)**

A paper from CSMD'S Future Technologies Group, titled "Opportunities for Nonvolatile Memory Systems in Extreme-Scale High Performance Computing" has been highlighted on HPCWire website . This paper discusses scaling challenges for DRAM and also explores the scope for emerging non-volatile memories, e.g. Flash, STT-RAM etc.

**Oak Ridge National Laboratory to Co-Lead DOE's New HPC for Manufacturing Program (September 24, 2015)**

Oak Ridge National Laboratory (ORNL) is collaborating with Lawrence Livermore and Lawrence Berkeley National Laboratories (LLNL and LBNL) on a new US Department of Energy (DOE) program designed to fund and foster public-private R&D projects that enhance US competitiveness in clean energy manufacturing.

"The Manufacturing Demonstration Facility has worked with numerous industry partners to overcome challenges in areas of advanced manufacturing, and ORNL is excited by the prospect of extending and accelerating this success through modeling and simulation," said John Turner, Group Leader for Computational Engineering and Energy Sciences and ORNL lead for HPC4Mfg. He added, "We look forward to collaborating with colleagues at LLNL and LBNL, and with industry partners, to apply our computational expertise to challenging clean energy manufacturing problems." Read the article [here]

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- Computational Earth Sciences
- Computational Engineering and Energy Sciences
- Computational Chemical and Materials Sciences
- Computational and Applied Mathematics
- Computer Science Research
- Future Technologies
- Scientific Data Group

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http://www.csm.ornl.gov/newsite/

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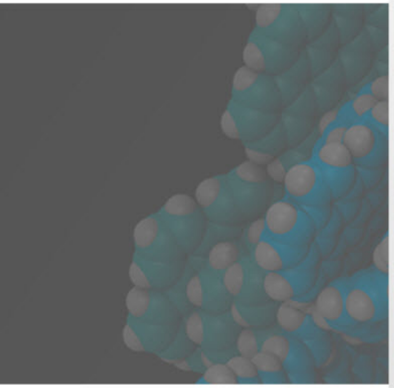

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## Computational Sciences and Engineering

**Deep Learning**

Deep learning (DL), a subset of machine learning, isdata driven feature extraction supported by hierarchical neuron layers. State of the art DL networks currently process data running on as many as 64 GPUs. Utilizing ORNL's DL expertise, we have created the Multi-node Evolutionary Neural Networks for Deep Learning (MENNDL) code running on ORNL's Titan supercomputer (containing more than 18,000 GPUs). This approach will discover both the optimal design parameters and topology of a deep learning network that will effectively remove the guesswork from the designing the optimal network. The optimal network can then be operated on smaller scale platforms.

**ORIGAMI**

ORiGAMI (Oak Ridge Graph Analytics for Medical Innovation) is a tool for discovering interesting associations and creating new testable hypotheses in medicine by "connecting the dots" across 70 million knowledge nuggets published in 23 million papers in the medical literature. The tool works on a 'Knowledge Graph' derived from SEMANTIC MEDLINE and integrated with scalable software that enables term-based, path-based, meta-pattern, and analogy-based reasoning principles. Use our demo-interface to explore your clinical questions and find answers to questions such as "How does Nexium treat Heartburn?" or "What are the viruses that have similar characteristics as Ebola?".

hypothesis.ornl.gov

**Cyber Security**

ORNL has developed and transitioned to private industry powerful new technologies for static analysis of compiled software (Hyperion) and prevention of data exfiltration (DataDiode). ORNL is currently developing advanced technologies that exploit physical properties to detect intrusions (Beholder) and to contain those intrusions (CICS), and to provide a platform that enables rapid technology prototyping, evaluation, and transfer that increases the potential cost to intruders while reducing the cost for defenders (the 1SR "shadow network").

www.cisr.ornl.gov

**Quantum Information Sciences**

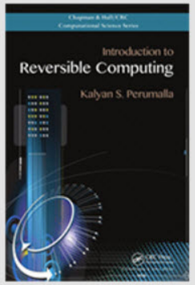
At the atomic scale, matter behaves according to the rules of quantum mechanics, leading to effects that are quite different than those that govern conventional logic gates. By exploiting these quantum phenomena, scientists hope to one day build a quantum computer that can perform certain computational tasks more efficiently than today's computers. Generating, managing, and reading information at the scale of a single atom is a formidable task, requiring the combined efforts of physicists, mathematicians, engineers, and computer scientists.

web.ornl.gov/sci/qis

**Reversible Computing**

What if: (i) Future hardware could recycle energy? (ii) Storage and retrieval to/from RAM becomes orders of magnitude slower than combinational logic? (iii) Blocked time in a parallel program dominates total time? Enter Reversible Computing as one of the most promising approaches to addressing all these questions at once. Researchers at ORNL have uncovered a critical role of reversible computing, especially focusing on its software-level aspects, and developed solutions ideal for addressing these challenges at extremely large parallel processing scales.

crcpress.com/Introduction-to-Reversible-Computing/Perumalla/9781439873403



# ORiGAMI

**Try ORiGAMI** | **Documentation - Interface**

**Try ORiGAMI API** | **Documentation - API**

ORiGAMI is a tool for discovering and evaluating potentially interesting associations and creating novel hypothesis in medicine. ORiGAMI will help you "connect the dots" across 70 million knowledge nuggets published in 23 million papers in the medical literature. The tool works on a 'Knowledge Graph' derived from SEMANTIC MEDLINE published by the National Library of Medicine integrated with scalable software that enables term-based, path-based, meta-pattern and analogy-based reasoning principles. We welcome you to use this tool (using our demo-interface or the API-interface) to explore your clinical questions and find answers to questions such as "How does Nexium treat Heartburn?", "What are the viruses that have similar characteristics as Ebola?", "Is xylene carcinogenic?", and "Can beta-blockers accelerate diabetic-retinopathy?".

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# DOE transforms HPC

OAK RIDGE NATIONAL LABORATORY

CSE Division CCS Directorate ORNL

# Quantum Information Science Group

Computational Sciences & Engineering Division

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- SPW 2013

## Welcome

The Quantum Information Science (QIS) group at the Oak Ridge National Laboratory applies the principles and techniques of quantum physics to real-world problems in communication, computing, and sensing. The sometimes surprising behavior of light and matter at the quantum level enables results that are simply not possible in the classical world. Our group carries out basic and applied research to identify and exploit these effects in order to realize the promises of QIS:

- In computing, quantum algorithms offer remarkable improvements in efficiency.
- The quantum properties of light provide privacy assurance and security guaranteed by the laws of physics.
- When applied to sensing, quantum approaches afford higher precision and faster acquisition.

Welcome CSE Division CCS Directorate ORNL Web Contact Disclaimer

Oak Ridge National Laboratory is a national multi-program research and development facility managed by UT-Battelle, LLC for the U.S. Department of Energy

UT-BATTELLE

U.S. DEPARTMENT OF ENERGY Office of Science

### NEWS AND EVENTS

New QIS group member: **Nicholas Peters** joined the QIS group on January 20, 2015. Nick earned a Ph.D. in Physics from the University of Illinois and has spent the past several years studying quantum communication in the telecommunications industry. Welcome to ORNL, Nick!

Congratulations to **Brian Williams**, who successfully defended his PhD thesis, "Nonlocal Polarization Interferometry and Entanglement Detection," at the University of Tennessee on November 7, 2014. Great job Dr. Williams! And a subsequent "Welcome to ORNL!" Brian joined the QIS group as a postdoc in December, 2014.

**QIS researchers have been awarded a grant** from the Cybersecurity for Energy Delivery Systems (CEDS) program in DOE's Office of Electricity. The three-year project, which is entitled "Timing Authentication Secured by Quantum Correlations," will combine quantum key distribution techniques with wireless communication to provide timing signals that are not subject to GPS spoofing. The project will be led by **Phil Evans**, and includes partners from PNNL, Sandia NL, Qubittek, Pacific Gas & Electric, and the University of Texas at Austin.

**New LDRDs: QIS researchers have been awarded FOUR new ORNL LDRD projects:**

http://web.ornl.gov/sci/qis/

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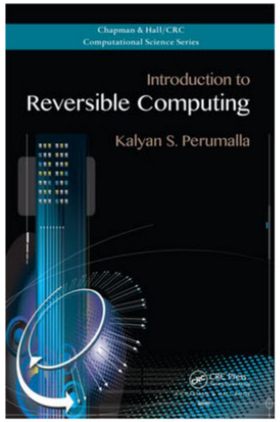


Preview this Book

Description
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Author(s) Bio

## Introduction to Reversible Computing

Kalyan S. Perumalla

Hardback $99.95 | eBook $69.97 | eBook Rental from $44.95

September 10, 2013 by Chapman and Hall/CRC
Reference - 325 Pages - 50 B/W Illustrations
ISBN 9781439873403 - CAT# K13404
Series: Chapman & Hall/CRC Computational Science

For Librarians — Available on CRCnetBASE >>

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### Features

- Emphasizes the software, programming, application, and usage aspects of reversible computing
- Helps readers easily understand complex theoretical and seminal results at a level suitable for senior undergraduate or graduate students
- Illustrates the development of reversible code generation using actual code segments in the C language
- Provides pseudocodes of several algorithms for memory-less or memory-efficient reversibility, including reversible random number generation and reversible numerical computation
- Includes a comprehensive bibliography and resources for further reading
- Offers source code for reversible random number generation and reversible models of abstract physical systems at www.rcbook.org

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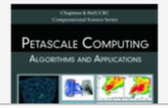


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OAK RIDGE National Laboratory

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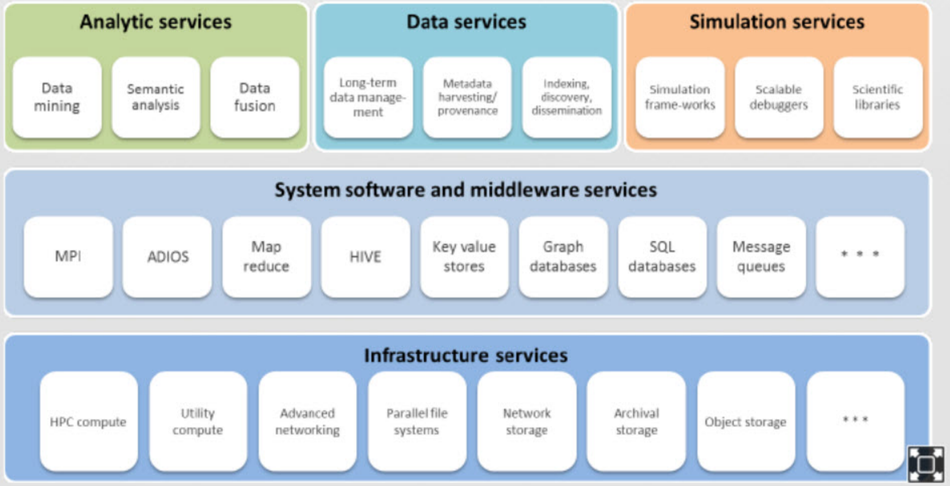
## CADES - The Compute and Data Environment for Science

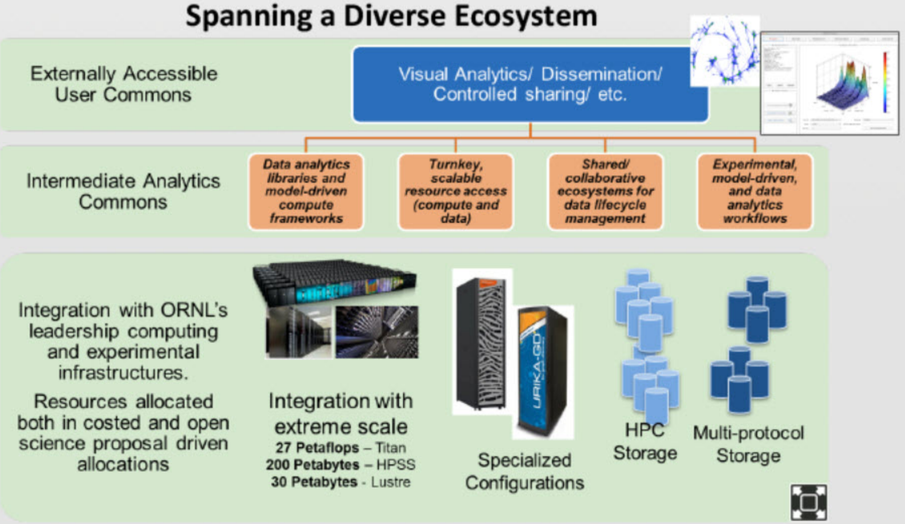
### Addressing the Big Data challenges at ORNL

- Facilities and research teams have increasing data analysis and data lifecycle management needs.
- Research teams are increasingly geographically distributed and require collaborative tools and shared access to data and analysis infrastructure.
- Research teams and facility users require access to and assistance from data science expertise to effectively conduct their research.
- CADES is designed to address these requirements by providing a flexible and adaptive computing and data infrastructure coupled with experts in data science to develop solutions.
- Exploits the observation that many Big Data projects have similar workflow needs: data fusion and reduction, streaming analysis, post analysis, and data curation and dissemination. Unifies *in silico* and *model-driven* exploration and *empirical* analysis.

### CADES Is Designed to Provide Individual Services and Integrated Workflows Solutions to Data Intensive Science Programs




### CADES Infrastructure Today: Analytics and Workflows Spanning a Diverse Ecosystem



## CADES Is Designed to Provide Individual Services and Integrated Workflows Solutions to Data Intensive Science Programs

**Analytic services**: Data mining | Semantic analysis | Data fusion

**Data services**: Long-term data manage-ment | Metadata harvesting/ provenance | Indexing, discovery, dissemination

**Simulation services**: Simulation frame-works | Scalable debuggers | Scientific libraries

**System software and middleware services**: MPI | ADIOS | Map reduce | HIVE | Key value stores | Graph databases | SQL databases | Message queues | * * *

**Infrastructure services**: HPC compute | Utility compute | Advanced networking | Parallel file systems | Network storage | Archival storage | Object storage | * * *

## CADES Infrastructure Today: Analytics and Workflows Spanning a Diverse Ecosystem

Externally Accessible User Commons: Visual Analytics/ Dissemination/ Controlled sharing/ etc.

Intermediate Analytics Commons: *Data analytics libraries and model-driven compute frameworks* | *Turnkey, scalable resource access (compute and data)* | *Shared/ collaborative ecosystems for data lifecycle management* | *Experimental, model-driven, and data analytics workflows*

Integration with ORNL's leadership computing and experimental infrastructures.

Resources allocated both in costed and open science proposal driven allocations

Integration with extreme scale
**27 Petaflops** – Titan
**200 Petabytes** – HPSS
**30 Petabytes** - Lustre

Specialized Configurations | HPC Storage | Multi-protocol Storage

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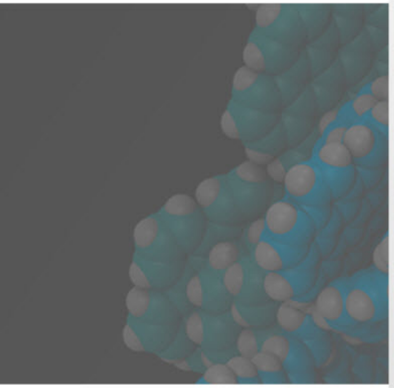

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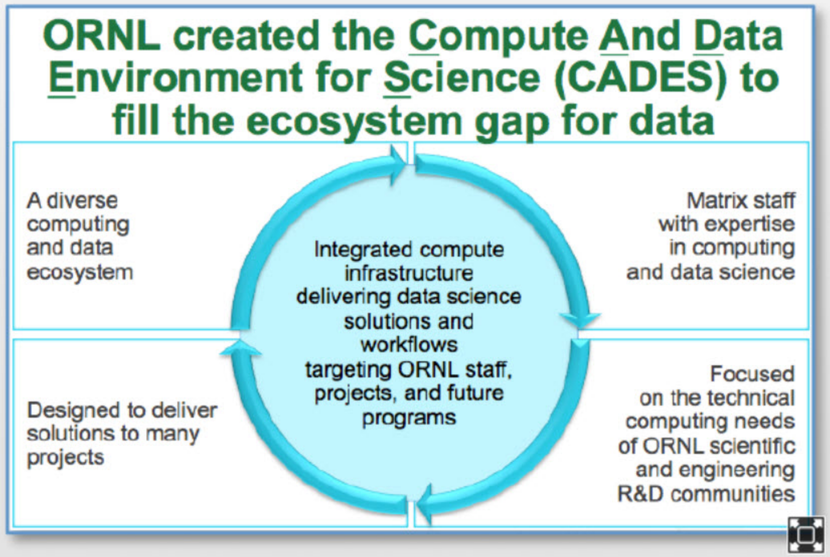
# Progress at ORNL of data pilot projects using CADES

Eleven DOE science data pilot projects were featured at the DOE lab booth at Supercomputing 2014. Of these eleven, seven leveraged capabilities of ORNL computing resources, including the Compute and Data Environment for Science (CADES). While each data pilot project had unique components of their workflow, common requirements emerged, many of which could only be met by building upon the scalable compute and data storage capabilities of CADES. In 2015, each project has continued their work, with a few key highlights detailed below.

"Big Data" is changing the way we do science across all domains:

- BIOLOGY
  Using large clusters, petabytes of storage, large memory platforms, and Map Reduce/ Hadoop systems, a collaboration between CADES, the Oak Ridge Leadership Computing Facility (OLCF), and biosciences is producing results. Big data and high performance computing are revealing the underlying biological signatures found in the measurement of single nucleotide polymorphisms (SNPs).
- CLIMATE
  The Accelerated Climate Modeling for Energy (ACME) collaboration has used big data workflows on CADES to increase the capability of running simulations and data management operations.
- MATERIALS
  Using CADES, the Institute for the Functional Imaging of Materials is enabling discovery through image analytics. Using scanning transmission electron microscopy, CADES quickly processes massive amounts of data into usable information on a workflow called BEAM.
- NEUTRONS
  The Center for Accelerated Materials Modeling at ORNL is using resources from CADES, the OLCF, and the Spallation Neutron Source, to conduct full scale *ab initio* molecular dynamics simulations on experiment timescale allowing real time decisions.

CADES

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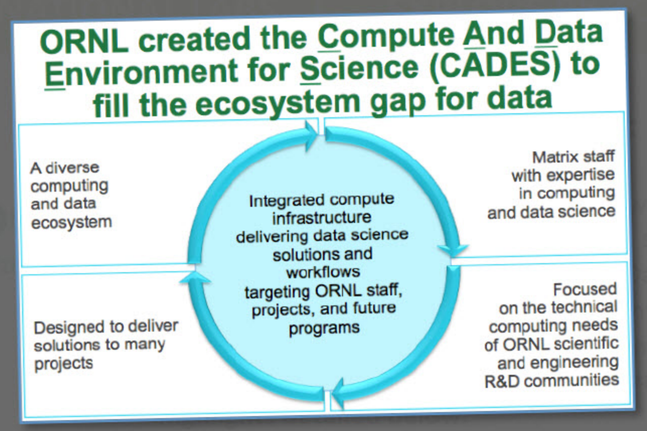


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National Lab

## data pilot projects using CADES

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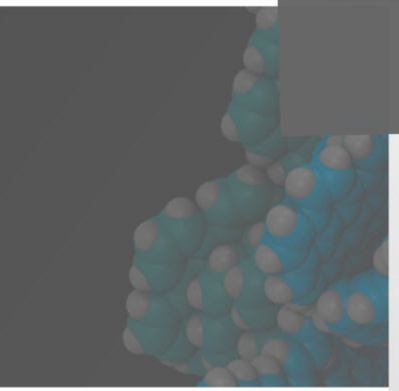
Arjun Shankar, CADES Director
shankarm@ornl.gov



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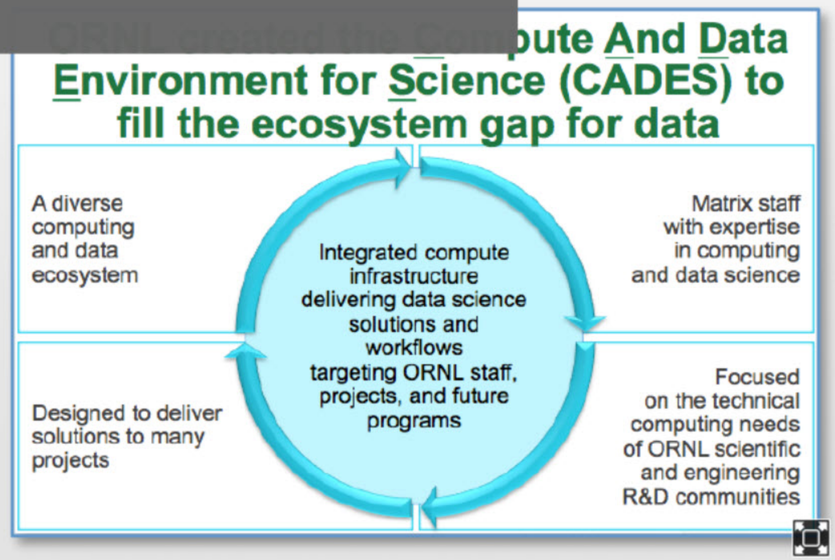


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OAK RIDGE National Laboratory

# Oak Ridge and Industry: Partnering for Success

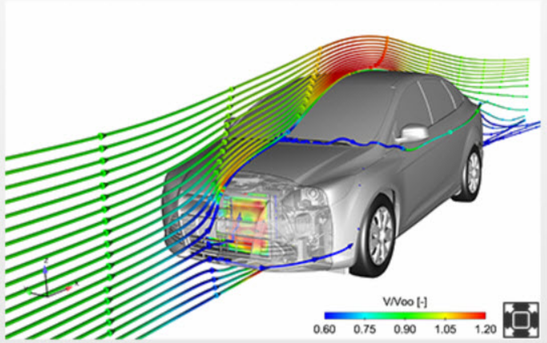
**What is ACCEL?**
*Accelerating Competitiveness through Computational ExceLlence* (ACCEL) is an Oak Ridge National Laboratory program helping companies supercharge their competitiveness through easy access to the lab's world class supercomputers and computational expertise.

**How are Companies Benefiting?**
- Successfully tackling strategic, competitively important problems that are too complex to solve with in-house computing resources.
- Reducing time to market for new products.
- Accelerating R&D and lowering its cost.
- Achieving breakthrough insights and understanding, and/or discovering something new.

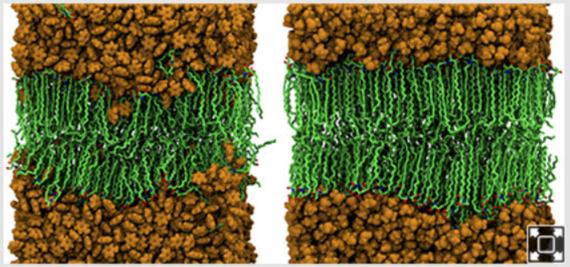
**Get in Touch and Explore the Possibilities!**

Suzy Tichenor
Director, Industrial Partnerships
tichenorsp@ornl.gov

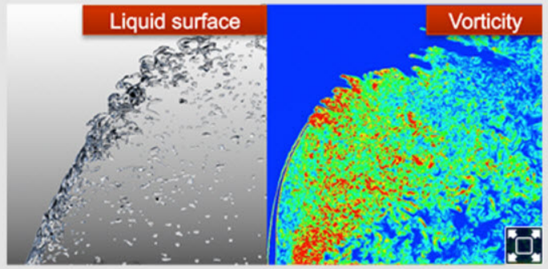
ACCEL
Accelerating Competitiveness through Computational ExceLlence




**FORD**
Visualization of vehicle cooling airflow optimized using advanced Design of Experiment-based CAE processes.



**Procter & Gamble**
Simulations of the upper most layer of skin, the stratum corneum (green), with additives (orange) phenol (left) and DMSO (right). Notice the high level of disruption on the case of phenol.




**United Technologies Research Center**
Spray atomization of liquid jet engine fuel.

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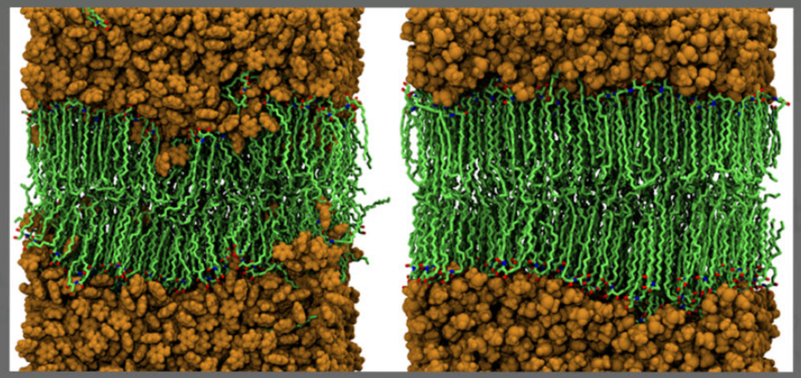
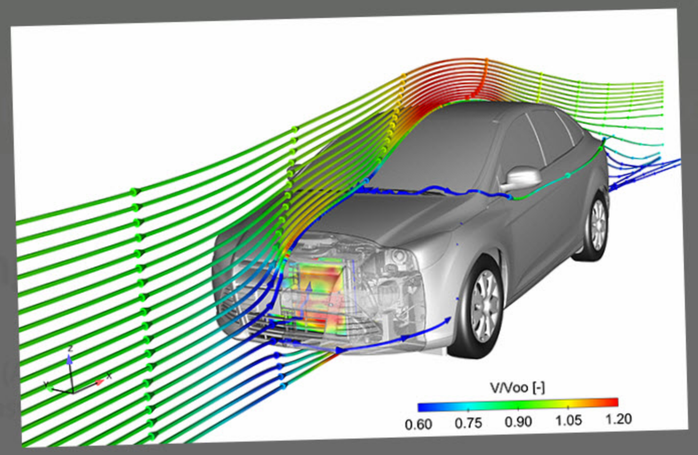


**Procter & Gamble**
Simulations of the upper most layer of skin, the stratum corneum (green), with additives (orange) phenol (left) and DMSO (right). Notice the high level of disruption on the case of phenol.




**FORD**
Visualization of vehicle cooling airflow optimized using advanced Design of Experiment-based CAE processes.

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Suzy Tichenor
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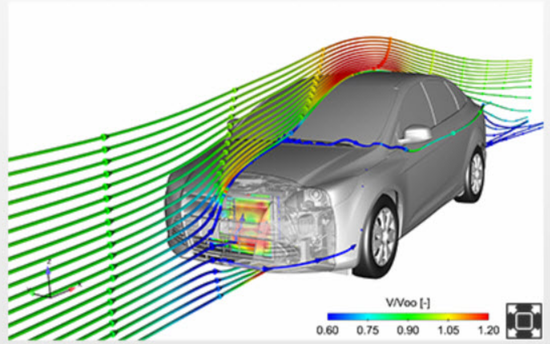


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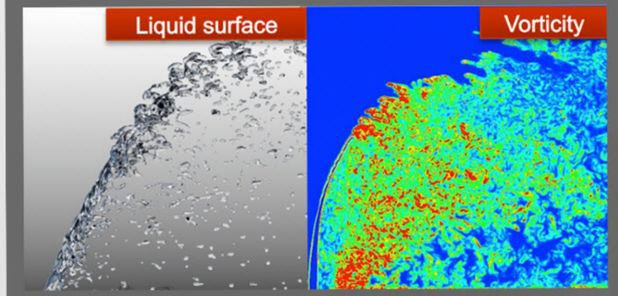
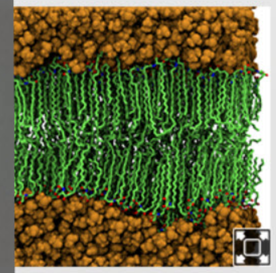



**United Technologies Research Center**
Spray atomization of liquid jet engine fuel.



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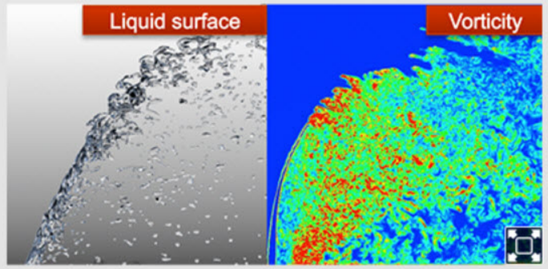


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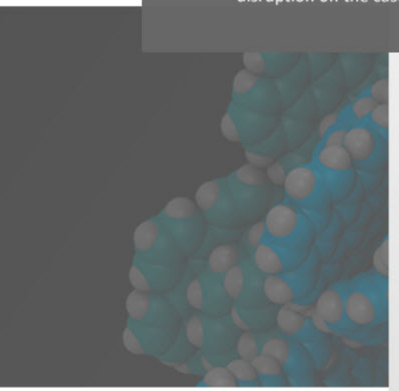

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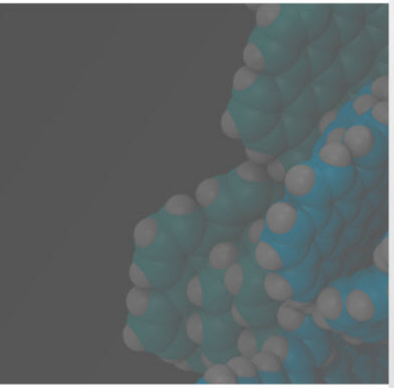

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# HPC at Oak Ridge National Laboratory's Institutes

As the US Department of Energy's largest multi-program laboratory, ORNL is engaged in a wide range of activities that support the department's mission of ensuring America's security and prosperity by addressing its energy and environmental challenges. To accomplish this, the laboratory applies a remarkable portfolio of scientific expertise and world-class scientific facilities and equipment to develop scientific and technological solutions.

The laboratory's major initiatives reflect an orientation toward both scientific disciplines and national missions, a combination that distinguishes ORNL and enables delivery of national-scale solutions to problems of critical importance. ORNL's Computing and Computational Sciences Directorate hosts or co-hosts several centers and institutes which are critical resources in the delivery of multidisciplinary science across the laboratory.

**Climate Change Science Institute (CCSI)**

*climatechangescience.ornl.gov*

A multidisciplinary research center established in 2009, the mission of the CCSI is to advance knowledge of the Earth system, describe the consequences of climate change, and evaluate and inform policy responses to climate change.

**Consortium for Advanced Simulation of Light Water Reactors (CASL)**

*www.casl.gov*

Established in 2010, CASL was DOE's first Energy Innovation Hub, which focuses on improving nuclear reactors through computer-based modeling.

**Health and Data Sciences Institute**

*hdsi.ornl.gov*

The HDSI at ORNL was established in 2013 to centralize all data-driven health science research and development activities. HDSI provides a collaborative R&D environment to enable scalable "big data"-driven biomedical innovation and transformation of healthcare.

**Institute for Functional Imaging of Materials (IFIM)**

*www.ornl.gov/science-discovery/advanced-materials/research-areas/institute-for-functional-imaging-of-materials*

IFIM is changing materials research by uniting experts in imaging instrumentation, fundamentals in physical and chemical imaging processes, and data analytics—accelerating the discovery, design, and deployment of new materials.

**Joint Institute for Computational Sciences (JICS)**

*www.jics.tennessee.edu*

JICS was established by the University of Tennessee and ORNL to advance scientific discovery and state-of-the-art engineering through modeling and simulation, with a focus on education of a new generation of researchers.

**Institute (UDI)**

*udi.ornl.gov*

Formed in 2014, the UDI uses scalable computing, data visualization, and unique data sets from a variety of sources to foster innovative interdisciplinary research that integrates ORNL expertise in energy, transportation, cyber, and data sciences.

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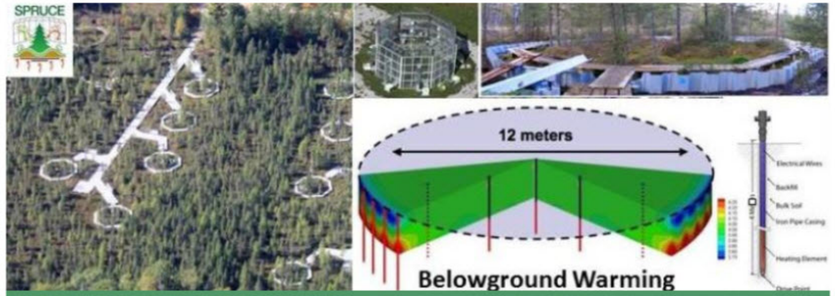

SPRUCE Research Site

## Current News

### Postdoctoral Research Associate Position - Linking root traits and ecosystem processes

The Environmental Sciences Division and the Climate Change Science Institute at Oak Ridge National Laboratory is seeking a postdoctoral research associate in the Terrestrial Ecosystem Science Program. Specific research tasks include woody plant fine-root and rhizosphere responses to warming and elevated [CO2] at a new climate change experiment in northern Minnesota, as well as linkages among root dynamics and ecosystem carbon and water fluxes in a long-running AmeriFlux site in Missouri. Focused, self-directed research is also expected.

http://climatechangescience.ornl.gov/

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CASL The Consortium for Advanced Simulation of LWRs
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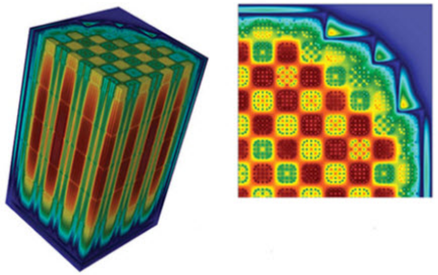

A 3D prediction of the power output, coolant temperature, and coolant density distribution within a PWR using coupled neutron transport and thermal-hydraulics options in Virtual Environment for Reactor Applications (VERA). The images illustrate the density of neutrons in the reactor at hot full power, where red represents a large density, yellow a moderate density, and blue a low density.

U.S. DEPARTMENT OF ENERGY

### SCIENCE AND TECHNOLOGY

**Energy Department Announces Five Year Renewal of Funding for First Energy Innovation Hub**
Consortium for Advanced Simulation of Light Water Reactors to Receive up to $121.5 Million Over Five Years.
Posted: January 29, 2015

**VERA-CS Coupled Multi-physics Capability demonstrated in a Full Core Simulation**
In December, CASL reported on the latest results from its Watts Bar reactor progression problem modeling.
Posted: August 14, 2014

**Westinghouse Completes its AP1000® Test Stand**
Last June, CASL launched its first Virtual Environment for Reactor Applications (VERA) Test Stand on the Westinghouse engineering computer cluster.
Posted on June 23, 2014

**University of Michigan adds Depletion Capability to MPACT for VERA-CS**
MPACT is a three-dimensional (3-D) whole core transport code being developed by the University of Michigan and ORNL for the CASL VERA toolset.
Posted on June 23, 2014

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- NURETH-16
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  Chicago, IL
- Coding for cooling: Benjamin Magolan helps model improved coolant flow

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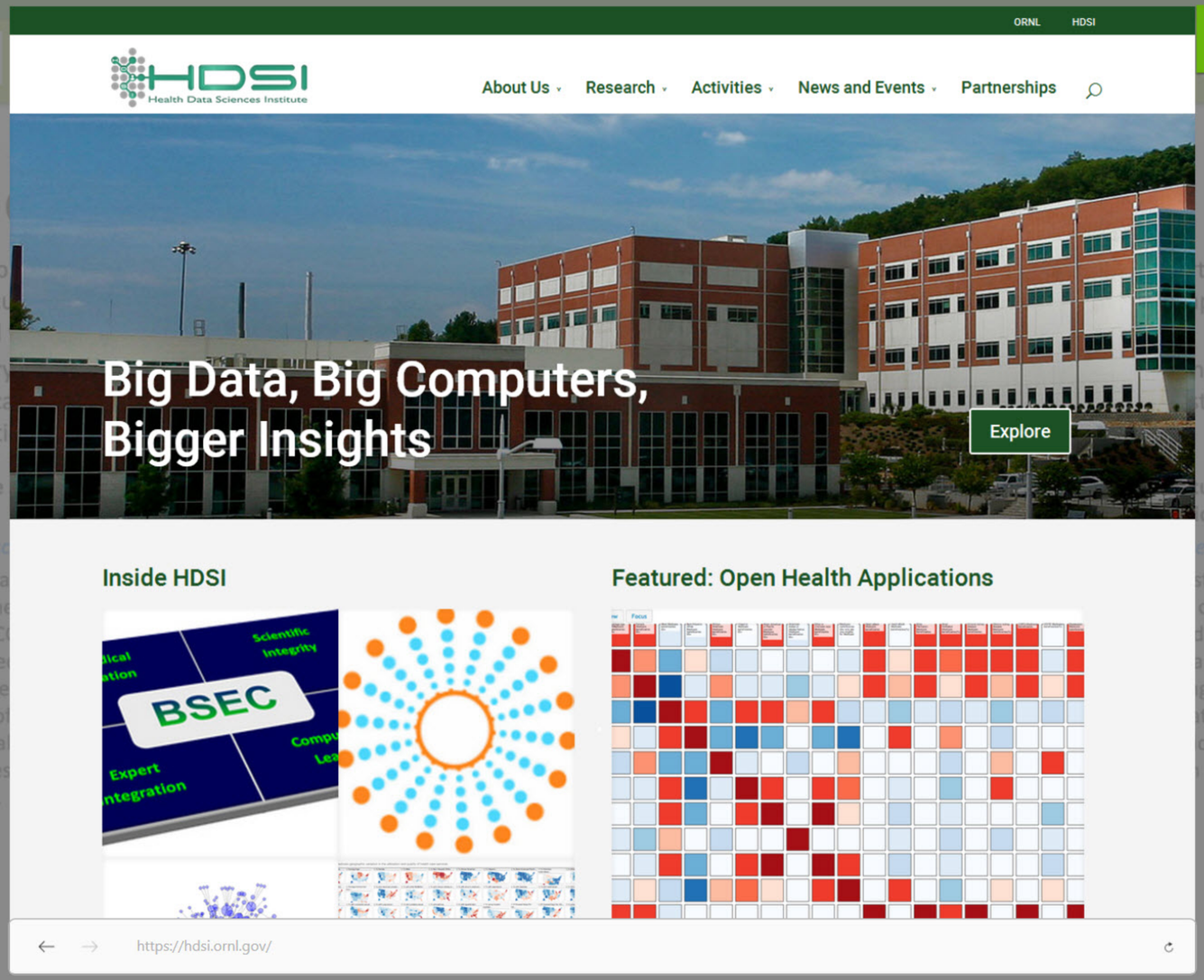
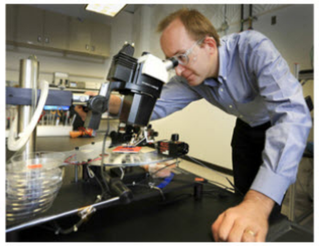


# Oak Ridge National Laboratory Launches Imaging Institute

June 23, 2014



*Sergei Kalinin is inaugural director of Oak Ridge National Laboratory's Institute for Functional Imaging of Materials. Image credit: Jason Richards, ORNL*

OAK RIDGE, Tenn., June 23, 2014—The Department of Energy's Oak Ridge National Laboratory has launched the Institute for Functional Imaging of Materials to accelerate discovery, design and deployment of new materials. The institute will meld world-class capabilities in imaging, high-performance computing, materials science and other scientific disciplines to probe materials. It supports President Obama's Materials Genome Initiative, which aims to bring new materials to the marketplace.

"Advanced materials are essential to clean energy, national security and global competitiveness," said ORNL Director Thom Mason. "Key energy technologies like solar cells, superconductors and batteries all have shortcomings that next-generation materials might overcome."

By focusing expertise from ORNL's diverse science portfolio, capabilities in high-performance computing, and success in creating new tools for discovery, the institute promises to speed the arrival of next-generation materials.

"In battery materials, for example, the grand challenge is looking at ions as they move and changes in electronic structure at the same time," said Associate Laboratory Director for Physical Sciences Michelle Buchanan. "We are bringing together leading researchers in imaging, computing and materials science to meet this challenge."

The new institute creates a focal point for ORNL's core capabilities. The national lab in Tennessee is home to several major DOE Office of Science user facilities, including America's fastest supercomputer, the world's most intense pulsed neutron beam and world-class facilities for electron/atom probe and scanning probe microscopy; mass spectrometry; and optical, X-ray and chemical imaging. Its Center for Nanophase Materials Sciences, Chemical Sciences Division and Materials Science and Technology Division provide state-of-the-art imaging capabilities. ORNL

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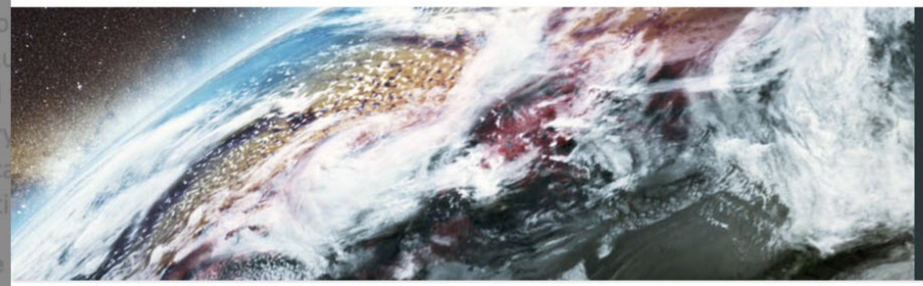

Advancing Discovery

## Technology

### Researcher Question and Answer

Ryan Glasby uses advanced computing to develop a computational fluid dynamics tool for customers that is robust and evolving to new computing architectures.

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### Ebola Article Earns Special Recognition

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