Science and Strategic Results
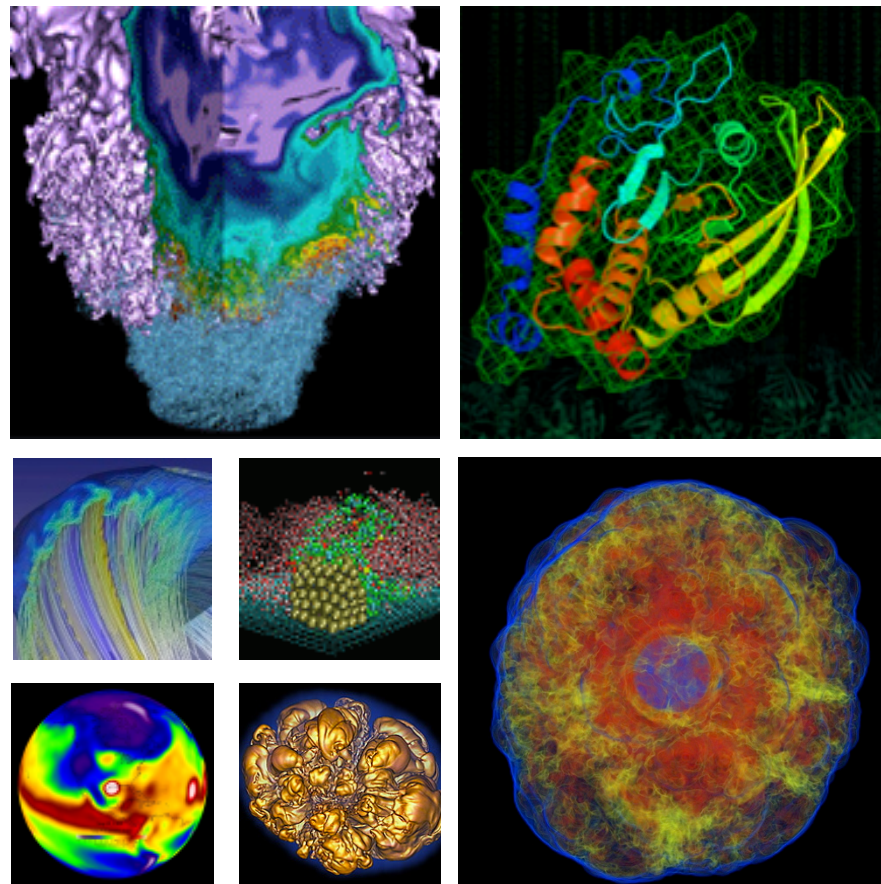
NERSC Operational Review 2016

February 16, 2016

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Charge Questions

Is the science output commensurate with NERSC's mission to "accelerate the pace of scientific discovery through high performance computing and data analysis"?

"Is NERSC optimizing the use of its resources consistent with its mission"?

Focus on Science

- **NERSC supports the broad mission needs of the six DOE Office of Science program offices**

- **6,000 users and 750 projects**

- **MPP (supercomputing) and data-only users**

- **NERSC science engagement team provides outreach and POC**

2,078 refereed publications in 2015
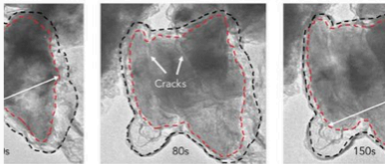
NERSC Science in the News

Social Media

Richard Gerber @ragerber 2d
#NERSC Coupling 2 'tabletop' laser-plasma accelerators: A step toward ultrapowe... bit.ly/20vcEoR via @BerkeleyLab @EurekAlertAAAS

Open

NERSC @NERSC 2d
RT @gizmag: Lithium-ion battery boost could come from "caging" silicon in graphene - gizm.ag/1Vye4M6 pic.twitter.com/dn5i0kdKhr


Open

Glenn K. Lockwood @glenn... 2d
NERSC hosting Advanced OpenMP workshop on Feb 4, led by members of OpenMP Lang Committee. Webcast avail, reg: nersc.gov/users/training...

NERSC's Impact on Advances of Global Gyrokinetic PIC Codes for Fusion Energy Research, Ethier, S. ; Choon-Seock Chang ; Seung-Hoe Ku ; Wei-li Lee ; Weixing Wang ; Zhihong Lin ; Tang, W.
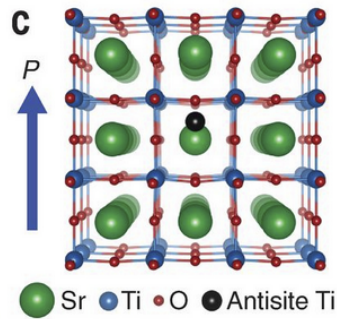
Big Bang, Big Data, Big Iron: Fifteen Years of Cosmic Microwave Background Data Analysis at NERSC, Borrill, J. ; Keskitalo, R. ; Kisner, T.

NERSC staff author book chapters on science accomplishments

NERSC Annual Reports
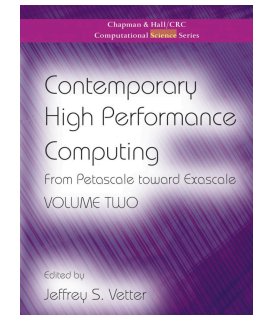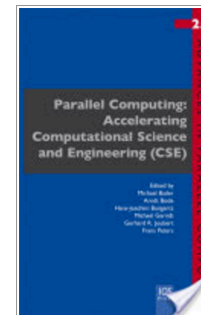
NERSC Sends Quarterly Highlights to DOE

C
P
Sr • Ti • O • Antisite Ti

Materials Science
Theoretical calculations help provide evidence of room-temperature ferroelectricity in nanometer-thick films **(Xifan Wu , Temple Univ., *Science*)**

Fusion Energy
3D simulations run at NERSC help gain new insights into fusion plasma behavior that will improve the ability to stabilize a tokamak reactor **(S. Jardin , Princeton Plasma Physics Lab, *Phys. Rev. Lett.*)**
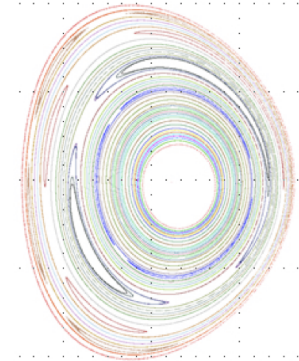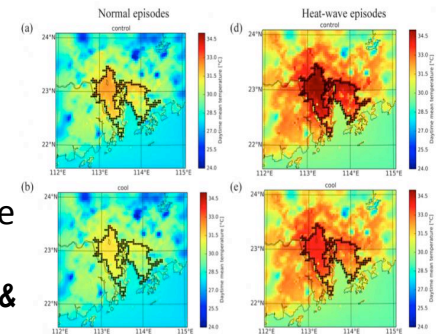

Chemistry
Simulations run at NERSC lead to the prediction of a new phase of superionic ice, a special form of ice that could exist on Uranus and Neptune **(Roberto Car , Princeton U., *Nature Comm.*)**
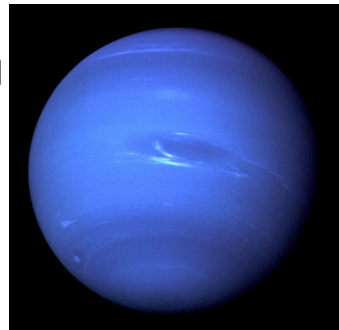
Energy
Computer models run at NERSC determine that, during a heat wave, white roofs can help mitigate the urban heat island effect **(Dev Millstein , LBNL, *Env. Sci. & Tech.*)**

High Energy & Nuclear Physics
Simulations run at NERSC are helping the Large Underground Xenon (LUX) dark matter experiment better focus their search for dark matter particles **(R. Jacobsen , LBNL, Phy. Rev. Lett.)**

Example Index Slide from December 2015
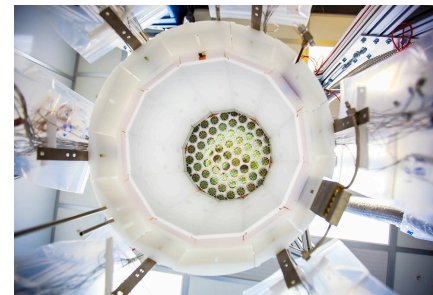
Selected Science Highlights
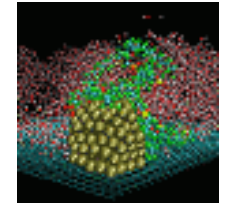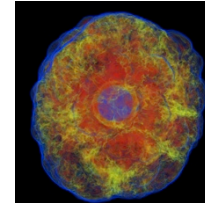
CT Scan of Earth Links Mantle Plumes with Volcanic Hotspots
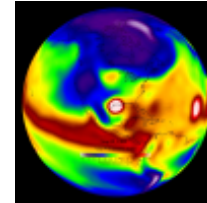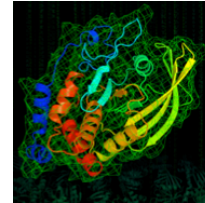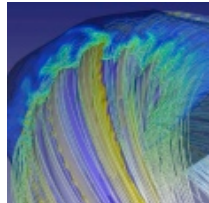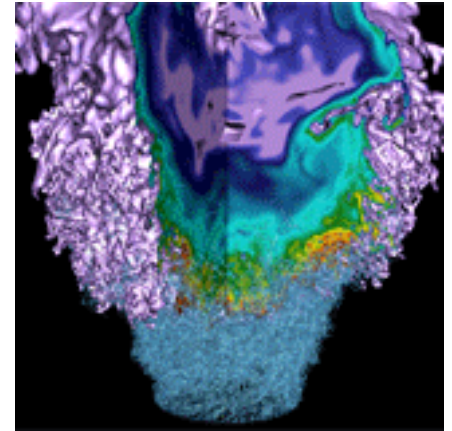
NERSC

Scientific Achievement

UC Berkeley seismologists produced the first a 3D scan of Earth's interior that conclusively connects plumes of hot rock rising through the mantle with surface hotspots that generate volcanic island chains.

Significance and Impact

Evidence for the plume and hotspot theory had previously been circumstantial; the theory has now been confirmed
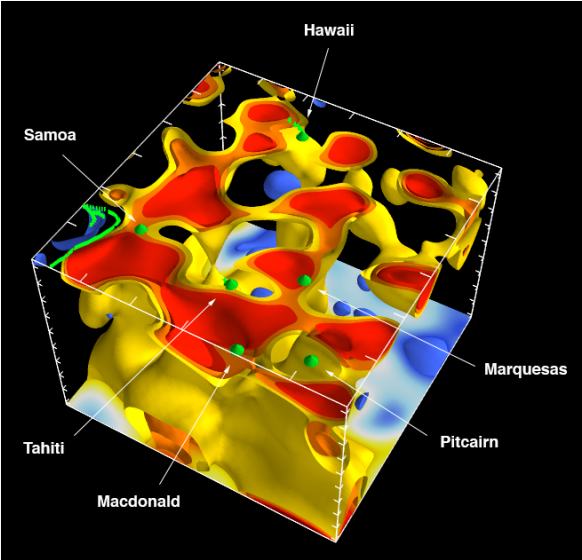
A 3D rendering of shear wave speed anomalies beneath the Central Pacific between the core-mantle boundary (2891 km depth) and 400 km depth. Green cones and labels highlight locations of key hotspot volcanoes in this region.

Novel programming tools: NERSC consultant and lead author Scott French wrote a data assimilation code that was one of the first to adopt UPC++ in production (distributed data structures supporting fast one-sided access / updates)

76 consulting tickets '12-'15 NERSC consultants helped with issues surrounding gasnet, Lustre striping, MPI IO

ERCAP Repo: m554
2014-15: 10.7 M hours used

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Nature 525, 95-99, Sep. 3, 2015.
French and Romanowicz, UC Berkeley

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Boosting Battery Research

Scientific Achievement

Demonstration that the solvation properties of two key electrolytes are governed by fundamentally different intermolecular interactions..

Significance and Impact

A central challenge in the refinement of lithium-ion batteries is to control cathode-induced oxidative decomposition of electrolyte solvents. This research, enabled by a new computational method, provided key insight regarding a central challenge in lithium-ion battery research: control of electrolyte decomposition

On the Cover: A plot showing the oxidized electron hole density distribution in two-molecules of ethylene carbonate.

NERSC NESAP Postdoc Taylor Barnes and lead author was a key contributor to the new "wave function-in-DFT" embedding approach that enables accurate calculation of ionization energy for individual solvent molecules at high accuracy while still accounting for bulk solvent effects using a combination of DFT and molecular mechanics interactions.. Approach was incorporated into December 2015 release of MOLPRO.

144 consulting tickets '12-'15 NERSC consultants helped with issues building and using applications: MOLPRO, CPMD, Gaussian, DL POLY, QChem

ERCAP Repo: m822 (Miller, Caltech)
2014-15: 33 M hours used

First Observations of a Supernova Colliding with its Companion

Scientific Achievement

A workflow enabled by a machine-learning data analysis pipeline developed in the Computational Research Division at LBNL and using NERSC computation, storage, and data analysis resources enabled the first ever observation of light from a supernova explosion debris slamming into a neighboring star.

Significance and Impact

Since Type Ia supernova serve as a key tool for measuring cosmic distances, a detailed understanding of this process is required to refine our understanding dark energy and the expansion of the universe.

ERCAP Repo: m937 (Nugent, UCB/LBNL)
2014-15: 500 K hours used
250 TB permanent disk storage
1.3 PB archival tape storage
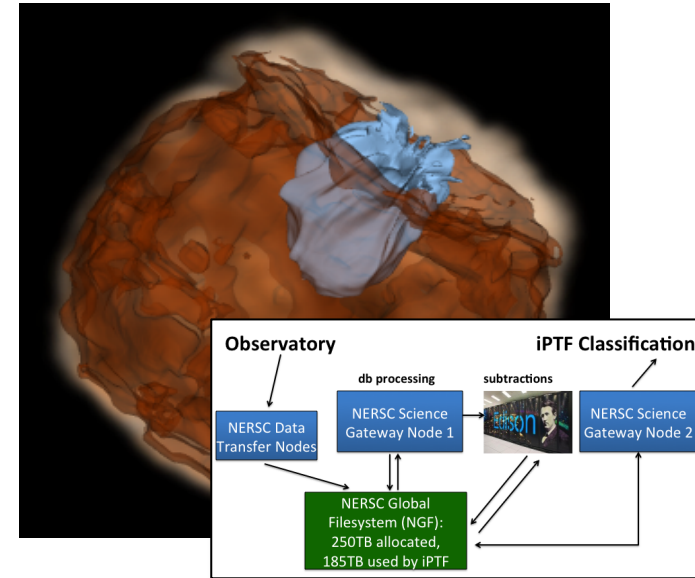
Simulation of the expanding debris from a supernova explosion (red) running over and shredding a nearby star (blue). Image: Daniel Kasen, LBNL/UCB. Inset: iPTF pipeline

415 consulting tickets '12-'15
The project used NERSC science gateways, databases, HTC queues, standing reservation. NERSC helped optimize python performance on HPC systems.

Stabilizing a Fusion Energy Plasma

Scientific Achievement

Using simulations run at NERSC scientists discovered that under certain conditions a helix-shaped whirlpool of plasma forms around the center of a tokamak fusion energy reactor that acts like a dynamo to help stabilize the plasma.
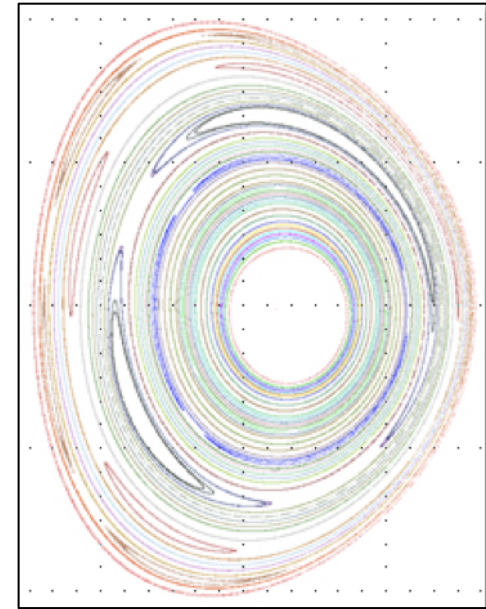
Significance and Impact

Scientists and engineers hope to be able to create these conditions on demand to stabilize "sawtooth" instabilities that would otherwise degrade the fusion process in reactors like the one being constructed at ITER multinational fusion facility in France.

NERSC consultant and NESAP contact Woo-Sun Yang has worked with S. Jardin and Intel to do in depth performance profiling of the M3D-C1 code. Yang has created an OpenMP enabled prototype of a M3D-C1 proxy code to help prepare the team for Cori.

ERCAP Repo: mp288 (Jardin, PPPL)
2014-15: 53 M hours used

A cross-section of the virtual plasma showing where the magnetic field lines intersect the plane.

315 consulting tickets '12-'15 NERSC consultants debugged numerous issues with M3D-C1 and PETSc.

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New Detailed View of Antarctic Ice Melt

NeRSC
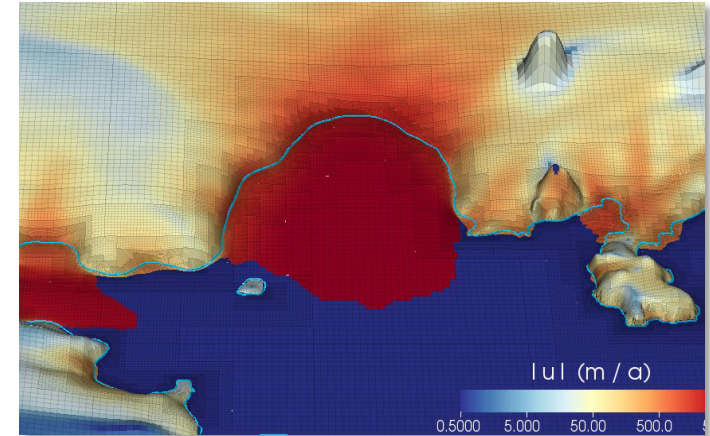
Scientific Achievement

A new high-resolution, large-scale computer model - Berkeley-ISICLES (BISICLES) - estimated how much ice the W. Antarctic Ice Sheet could lose over the next two centuries and how that could impact sea-level rise.

Significance and Impact

The acceleration of West Antarctic ice streams in response to ocean warming could result in a major contribution to sea-level rise, but previous (lower resolution) models were unable to quantify this.

Computational scientists at LBNL, including NERSC's Woo-Sun Yang, formed a collaboration with climate scientists at LANL and the University of Bristol, which led to the development of BISICLES.

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0.5000   5.000   50.00   500.0

Computer simulations run at NERSC show estimates of ice retreat in the Amundsen Sea Embayment by 2154. West Antarctica is one of the fastest warming regions on Earth, and its ice sheet has seen dramatic thinning in recent years. The ice sheet is losing significant amounts of ice to the ocean, with the losses not being offset by snowfall.

389 consulting tickets '12-'15 NERSC consultants helped debug problem with static vs. dynamic linking of the code.

ERCAP Repo: m1041 (Martin, LBNL)
2014-15: 10.4 M hours used

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S.L. Cornford, D. Martin et al
The Cryosphere, 9, 1579-1600, 2015

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Petascale Pattern Recognition for Climate Science

Accomplishments

- Modern climate simulations produce massive amounts of data, requiring sophisticated pattern recognition algorithms.

- The Toolkit for Extreme Climate Analysis (TECA) was developed at Berkeley Lab to help researchers detect extreme weather events in large (petabyte- to terabyte-sized) datasets

- The team downloaded 56 TB of climate data from the 5th phase of the Coupled Model Intercomparison Project to NERSC toidentify 3 classes of storms: tropical cyclones, atmospheric rivers and extra-tropical cyclones.

- NERSC's Hopper Cray XE6 system was used to preprocess the data, which took about two weeks and resulted in a final 15 TB dataset

- TECA: Petascale Pattern Recognition for Climate Science," presented at the 16th International Conference on Computer Analysis of Images and Patterns, was awarded the Juelich Supercomputing Center prize for the best application of HPC technology in solving a pattern recognition problem

Using TECA on NERSC's Hopper system and Argonne's Mira system reduced the runtime for pattern detection tasks in large climate datasets from years to hours

598 consulting tickets '12-'15 NERSC's Prabhat is a key member of the team responsible for the development of novel TECA

ERCAP Repo: m1517 (O'Brien, LBNL)
2014-15: 71 M hours used
Permanent Disk: 110 TB
Archival Storage: 5 PB

Assessing Environmental Impact of 'Fracking' on Drinking Water

Accomplishments

- Hydrocarbon production from unconventional resources and the use of reservoir stimulation techniques such as hydraulic fracturing ("fracking") has grown explosively over the last decade. But there are concerns that reservoir stimulation may create significant environmental threats

- To assess the potential impact of fracking on drinking water resources, environmental researchers ran a series of numerical simulations on NERSC's Hopper and Edison systems

- They found that, except for a brief initial period of upward flow during the initial phase of rapid gas ascent in the connecting feature (if such gas is present), water flow is uniformly downward

- These findings support a 2015 EPA study that concluded that below-ground migration of liquids and gases have not led to widespread impact on U.S. drinking water resources
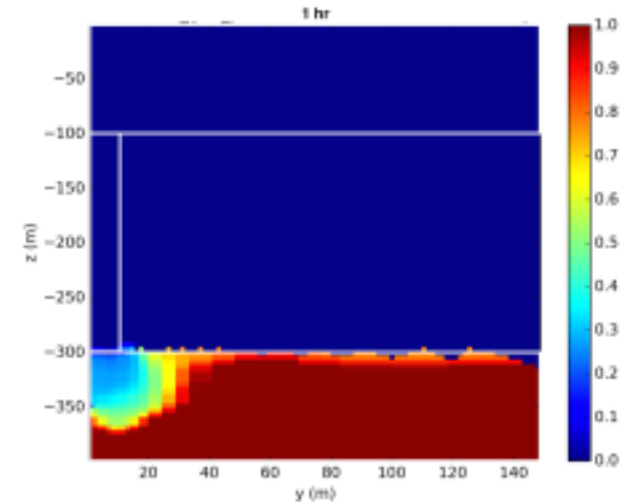
Gas phase saturation (S_G) in the plane of the connecting fracture at t = 1.0 hour

Repo: m1492 (Moridis, LBNL) 2014-15: 1.8 M hours used

98 consulting tickets '12-'15 NERSC's Prabhat is a key member of the team responsible for the development of novel TECA

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LUX Dark Matter Experiment

Scientific Achievement

Simulations run at NERSC are helping the Large Underground Xenon (LUX) dark matter experiment help rule out the possibility of dark matter detections at low-mass ranges where other experiments had previously reported potential detections

Significance and Impact

- LUX researchers are looking for WIMPs (weakly interacting massive particles), which are among the leading candidates for dark matter
- Improvements in LUX calibration, coupled with computer simulations run on NERSC's Edison supercomputer, allowed scientists to test additional particle models of dark matter that now can be excluded from the search
- NERSC also stores large volumes of LUX data—measured in trillions of bytes (terabytes)—on an ongoing basis.

ERCAP Repo: lux (Jacobsen, LBNL)
2014-15: 300 K hours
Permanent Disk : 30 TB
Archival Data: 250 TB
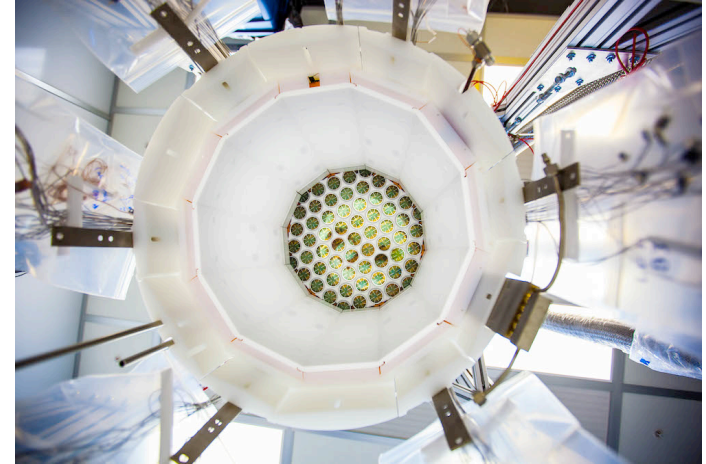
A view inside the LUX detector.

388 Consulting Tickets '12-'15 NERSC staff worked with LUX scientists to develop analysis on SciDB, a parallel database at NERSC. Together they designed a set of key SciDB queries that were able to produce results in hours rather than days.

LUX Collaboration,
Phys. Rev. Lett., Dec. 11, 2015

Polarized Laser Pulses Could Change Nature of Graphene

NeRSC

Scientific Achievement

Simulations run at NERSC show that hitting graphene with realistic low-frequency circularly polarized laser pulses can cause it to change state from a semi-metal to an insulator.

Significance and Impact

Graphene could be used to replace traditional semiconductors to encode and store information, with possible applications in low-energy electronics, quantum computing, light detectors …

Further Details

The results showed that the "handedness" of the laser pulses led to interesting and unexpected properties: not only does it produce a band gap, but it also induces a quantum state that can be switched either "on" or "off."

Repo: m974 (Derereaux, SLAC)
2014-15: 1.8 M hours used
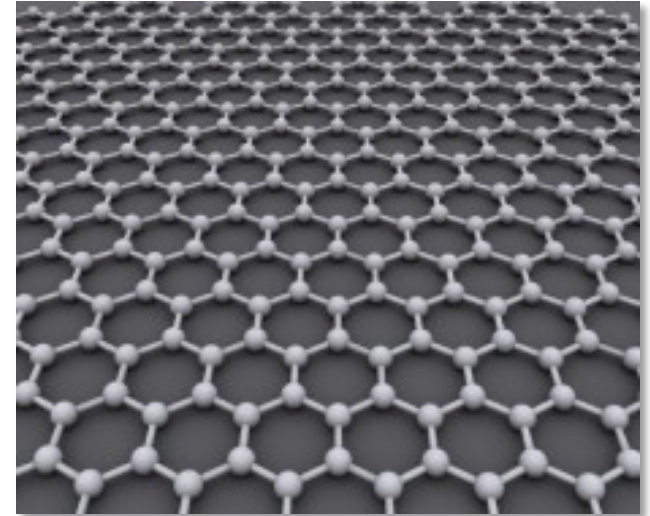
This illustration depicts the structure of graphene, which consists of a single layer of carbon atoms arranged in a honeycomb pattern. A new simulation suggests that spiraling pulses of polarized laser light could change graphene's nature, turning it from a metal to an insulator.

45 consulting tickets '12-'15 NERSC consultants helped track down errors when using the complex eigensolver with the PARPACK libraries on Hopper.

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# Nobel Prize in Physics 2015

Scientific Achievement

The discovery that neutrinos have mass and oscillate between different types

Significance and Impact

The discrepancy between predicted and observed solar neutrinos was a mystery for decades. This discovery overturned the Standard Model interpretation of neutrinos as massless particles and resolved the "solar neutrino problem"

Research Details

The Sundbury Neutrino Observatory (SNO) detected all three types (flavors) of neutrinos and showed that when all three were considered, the total flux was in line with predictions. This, together with results from the Super Kamiokande experiment, was proof that neutrinos were oscillating between flavors and therefore had mass
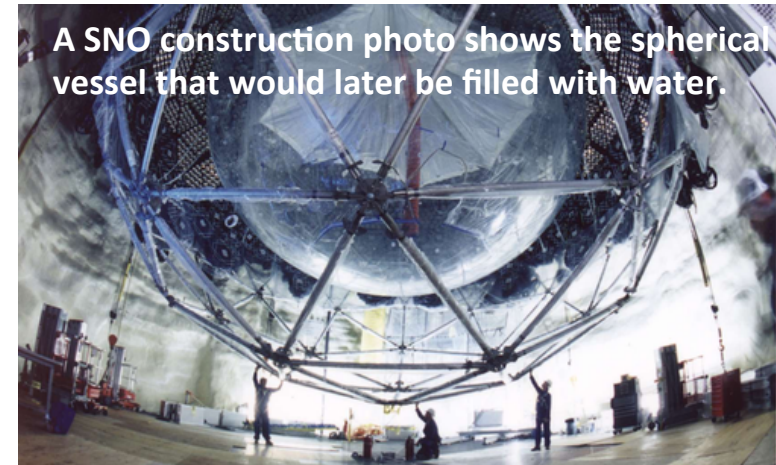
A SNO construction photo shows the spherical vessel that would later be filled with water.

Calculations performed on PDSF & data stored on HPSS played a significant role in the SNO analysis. The SNO team presented an autographed copy of the seminal *Physical Review Letters* article to NERSC staff.

Q. R. Ahmad et al. (SNO Collaboration). Phys. Rev. Lett. 87, 071301 (2001)

Nobel Recipients: Arthur B. McDonald, Queen's University (SNO)
Takaaki Kajita, Tokyo University (Super Kamiokande)
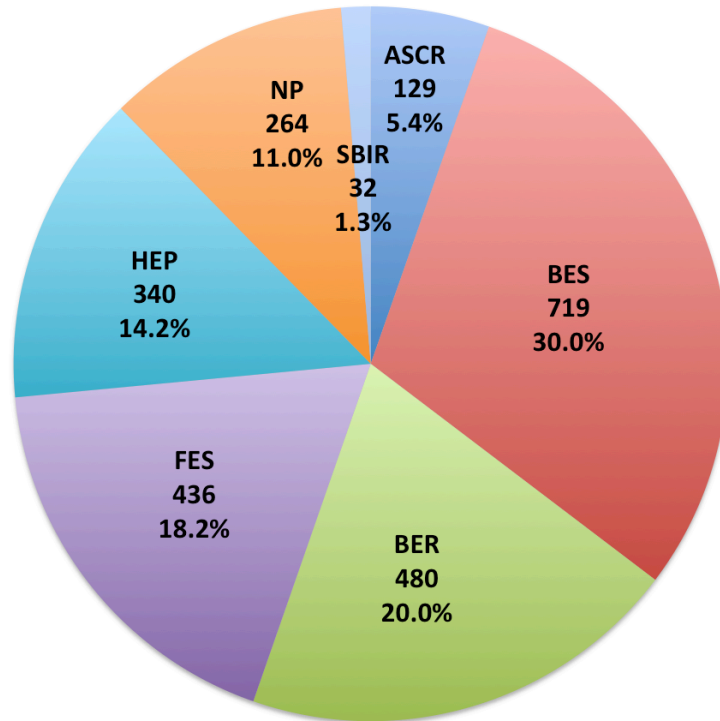
Allocation Pools and Usage

- **NERSC commitment to DOE in AY2015: 3 Billion MPP Hours**
  - 2,400 M for DOE Production (mission computing)
  - 300 M for ALCC (ASCR Leadership Computing Challenge)
  - 300 M for NERSC Director's Reserve
- **Additional time set aside for miscellaneous: ~54 M**
  - NERSC overhead
  - Education
  - Startup accounts
  - Vendors
- **Additional time is available if system downtime less than estimated or new resources become available (e.g. preproduction systems)**

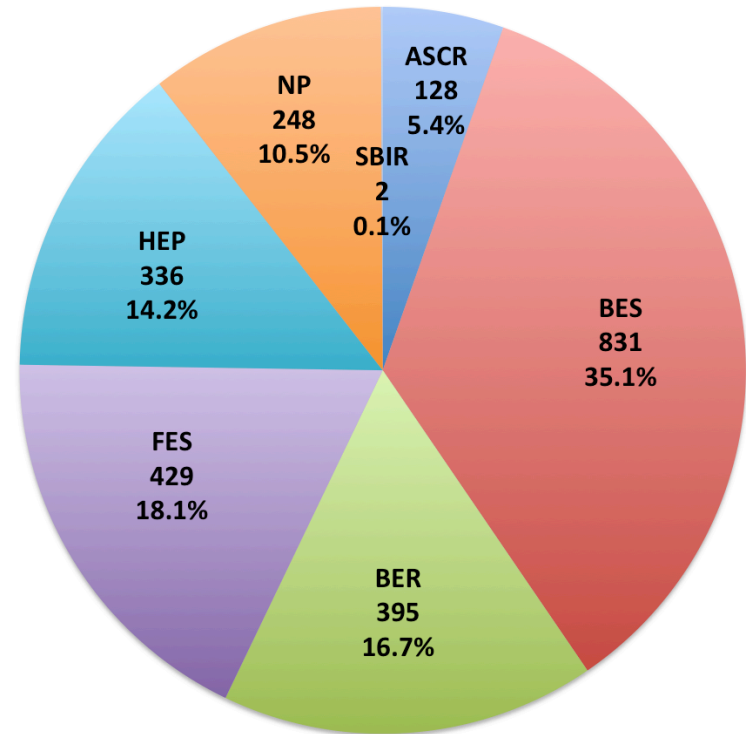# 2015 DOE Production Allocations and Usage by OSC Program Office

Allocation

Initial Allocation of Hours by DOE OSc Program Office 2015

- ASCR 129 5.4%
- SBIR 32 1.3%
- BES 719 30.0%
- BER 480 20.0%
- FES 436 18.2%
- HEP 340 14.2%
- NP 264 11.0%

2,400 M Hours

MPP Hours ~~Used~~ Charged

2015 Hours Used (Million MPP Hours)

- ASCR 128 5.4%
- SBIR 2 0.1%
- BES 831 35.1%
- BER 395 16.7%
- FES 429 18.1%
- HEP 336 14.2%
- NP 248 10.5%

2,777 M Hours Used

2,368 M Hours Charged

2015 Survey Responses by OSC Program Office

Number of Survey Respondents by DOE Office

ASCR 5.4%
SBIR 0.1%
NP 10.5%
HEP 14.2%
BES 35.1%
FES 18.1%
BER 16.7%
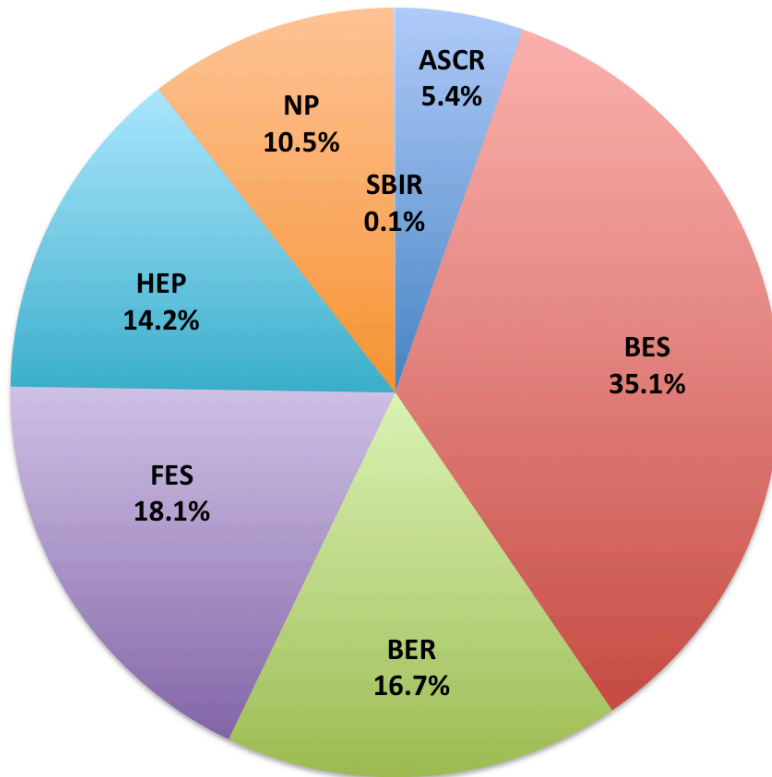
Survey Respondents by DOE Office by Hours Used

NP 15.9%
ASCR 16.5%
HEP 15.7%
BES 20.8%
FES 17.3%
BER 13.7%
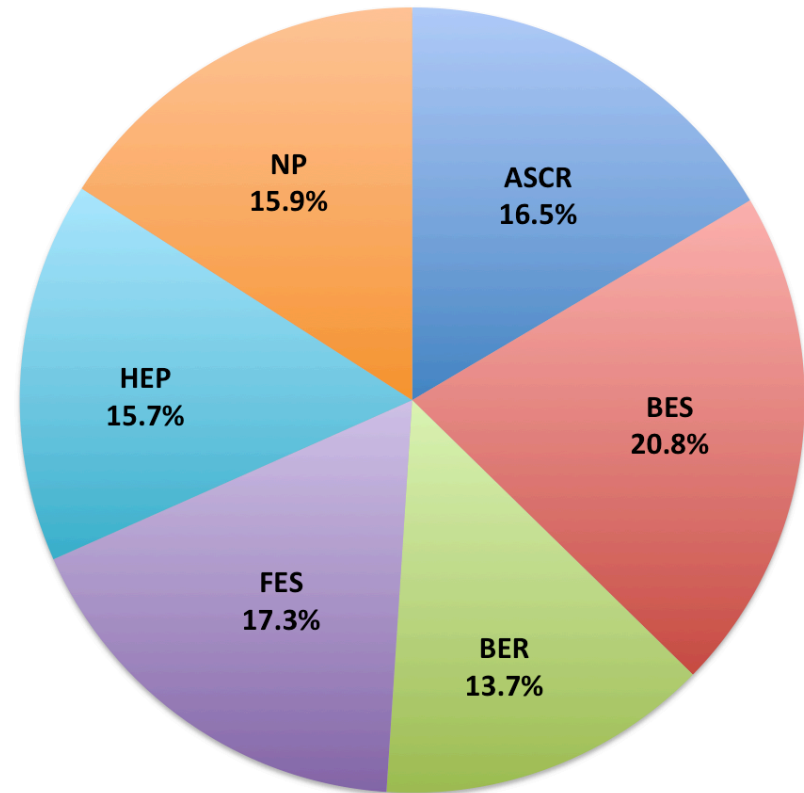
Hours Used Relative to DOE Base Allocation
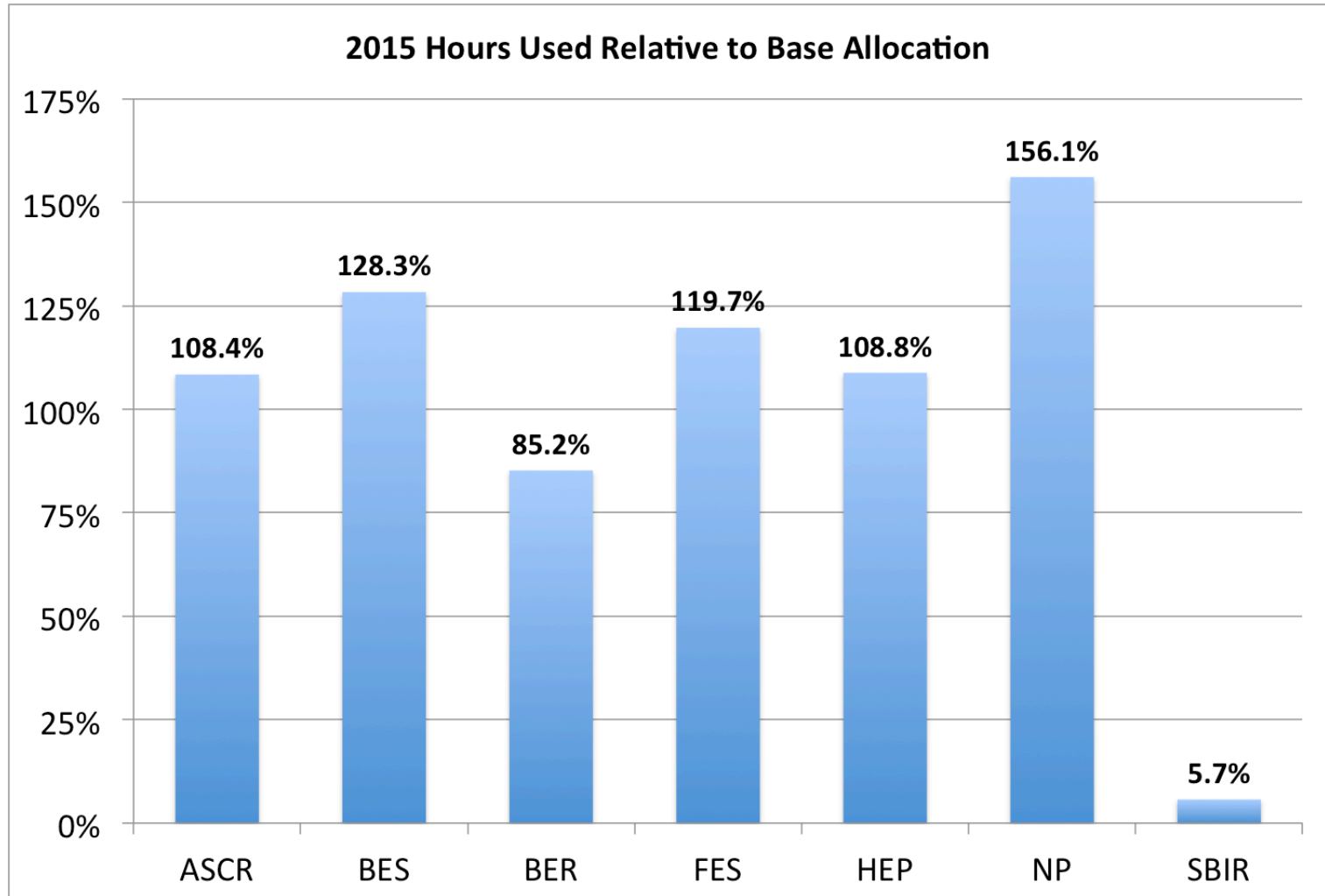
Division Director's Reserve Supports Strategic Programs and High-Impact Science

Category	Number of Projects	Allocated from DDR (Millions of MPP Hours)
Director's Reserve Projects	45	161
Additional Support for High-Impact Mission Science	221	139
TOTAL		**300**

Many DDR Projects supported science that doesn't neatly fit into an Office of Science office mission and scientific computing/data research and engineering, and industrial partners

- Anchored Solar-Driven Vortex for Power Generation, U. Illinois
- XPRESS Program Environment Testing at Scale, Sandia
- Atomic-Scale Modeling of Fracture Along Grain Boundaries with He, Kinetrics, Inc.
- Integrated Tools of Next-Generation Bio-Imaging, LBNL
- High Performance Flux Prediction Towards Radiological Resilience, LBNL
- Greening the Grid USAID/India, LBNL
- Traleika Glacier X-Stack, Intel
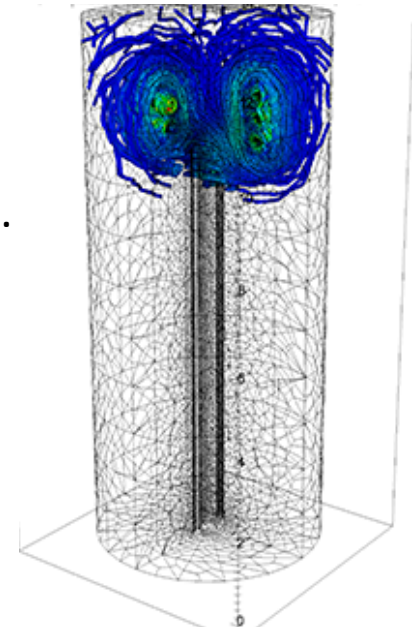
Industrial Partnerships

- **Separate SBIR allocation pool now in place**

- **130 industry users**

- **50 companies**

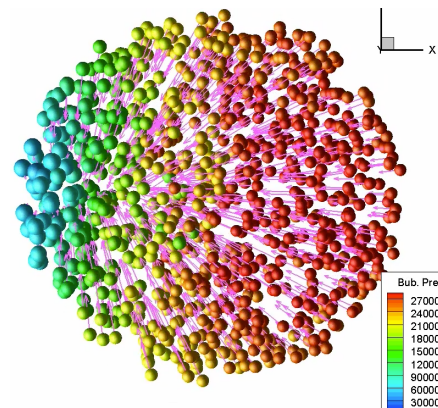- **Added 9 new projects in energy-specific fields in 2015**

Vertum Partners

Tech-X, Inc.

DynaFlow, Inc.

Bub. Pres.
270000
240000
210000
180000
150000
120000
90000
60000
30000

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Supercomputers and the Future of Wind Energy

NeRSC

Scientific Achievement

Success in simulations to assess impact of complex terrain on wind turbine efficiency is now leading to assessment of climate change and lightening effects on wind power production and revenue.

Significance and Impact

Electric utilities are keenly interested in evaluating the effects of climate change and extreme weather on wind energy.

Research Details

- Uses the WRF code to solve a 4D model of the atmosphere, including all basic dynamics and energy equations, while allowing for targeted parameterizations and interaction with the land and water bodies.
- NERSC resources allow evaluation of the sensitivity of the model results to different land surface types, atmospheric datasets and other forcings both internal and external to the model.

VertumPartners

This work has been using **4-D next-generation mesoscale numerical weather simulations** that model complex atmospheric data resolved to local wind farm scales. This will allow for optimal turbine site selection and evaluating the true climate change effects to wind energy.

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New Industrial Partners for 2015

| Company	Area of Research
Chemical Semantics, Inc.	Materials science
Civil Maps	Monitoring of energy infrastructure
Cymer Inc.	EUV lithography
Exabyte	Materials science
Global Foundries	Semiconductor design & fab
Kinectrics	Metal alloys for pipe networks
Melior Innovation	Geothermal reservoirs
Nano Precision Products	Optical interconnects
Quantumscape	Solid-state batteries for electric cars

Superfacility Concept
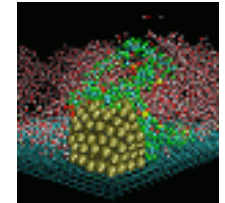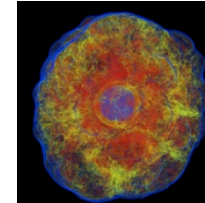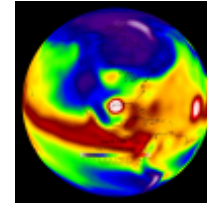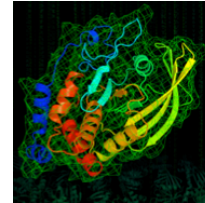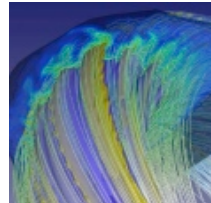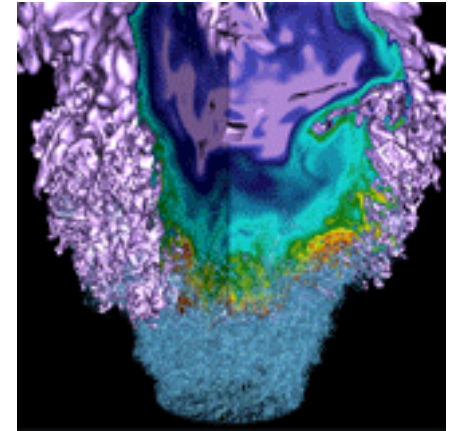
Experimental and observational science is at crossroads
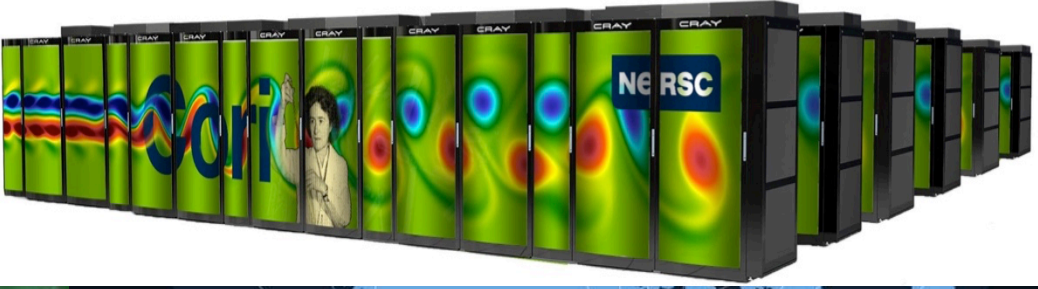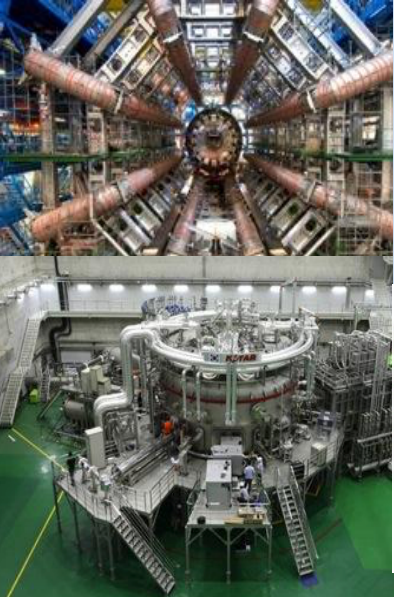
- **Data volumes are increasing faster than Moore's Law**

- **New algorithms and methods for analyzing data**

- **Infeasible to put a supercomputing center at every experimental facility**
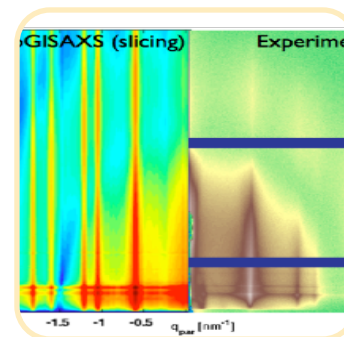
Computing Sciences Area
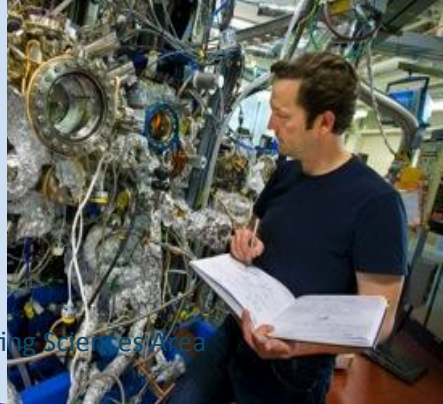
Superfacility Prototype and Use Case :
Process of science transformed

'Eliminate boundaries between the Scientist and the world's best algorithms running on the best architecture for that code'

Real-time analysis of 'slot-die' technique for printing organic photovoltaics, using ALS + NERSC (SPOT Suite for reduction, remeshing, analysis) + OLCF (HipGISAXS running on Titan w/ 8000 GPUs).

http://www.es.net/news-and-publications/esnet-news/2015/esnet-paves-way-for-hpc-superfacility-real-time-beamline-experiments/ Results presented at March 2015 meeting of American Physical Society by Alex Hexemer. Additional DOE contributions: **GLOBUS** (ANL), **CAMERA** (Berkeley Lab)

Computing Sciences Area

Answer to Charge Question

Is the science output commensurate with NERSC's mission to "accelerate the pace of scientific discovery through high performance computing and data analysis"?

- Yes, 2,078 publications in 2015; many in high-impact journals like Nature, Science, Phys. Rev.
- Yes, NERSC effectively supports 6,000 users and 750 projects
- NERSC significantly grew the industrial partnerships program in 2015
- NERSC is supporting high-impact scientific discovery from its partnerships with experimental facilities
- NERSC staff are actively involved in helping science teams make significant to scientific discoveries

Answer to Charge Question

Is NERSC optimizing the use of its resources consistent with its mission? Yes.

- NERSC delivered over the committed 3B hours to DOE users for a total of 3.17B hours

- The NERSC Director's reserve is managed effectively, with allocations going to high priority Office of Science projects and new strategic projects

Thank you.