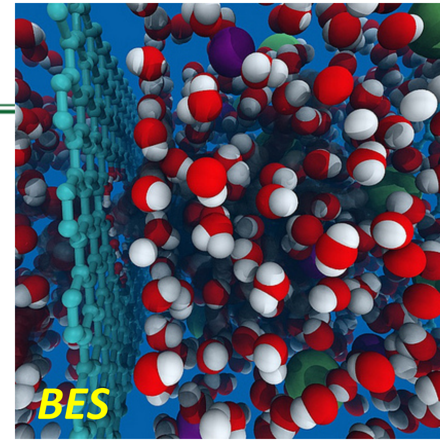
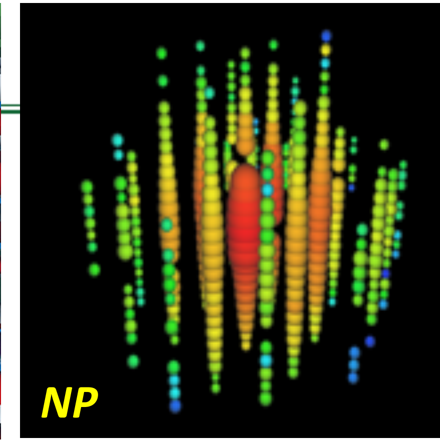
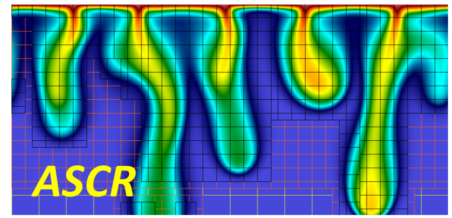
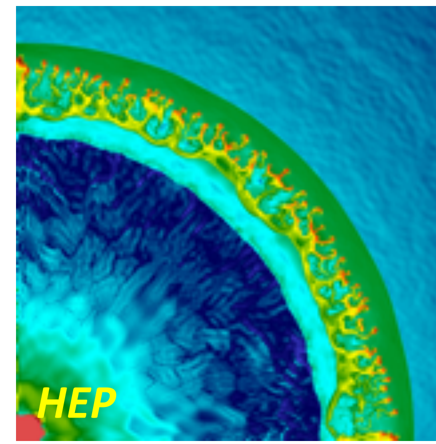
NERSC Science Highlights

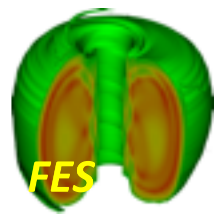
March 2016

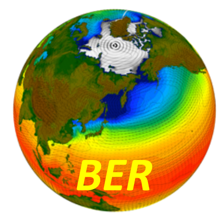












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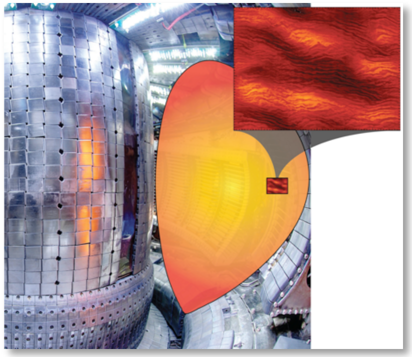
Science Highlights March 2016



Fusion Energy

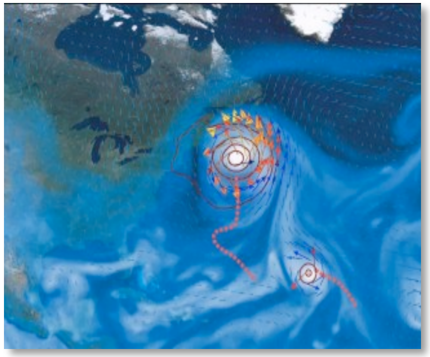
Results explain the mismatch between predictions and observations of heat loss in tokamak reactors.

(Howard, MIT, *Nuclear Fusion*)

Climate

Researchers have reduced the time needed to detect important features in large climate datasets from years to hours.

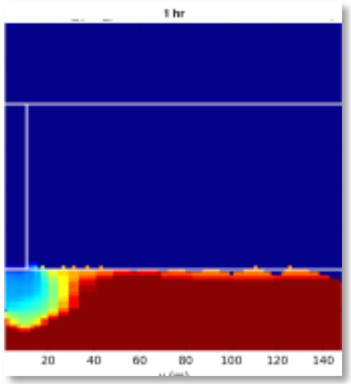
(O'Brien, LBNL. Env. Sci. & Tech)



Energy & Environment

Simulations support findings that migration of liquids and gases due to fracking have not had a widespread impact on drinking water.

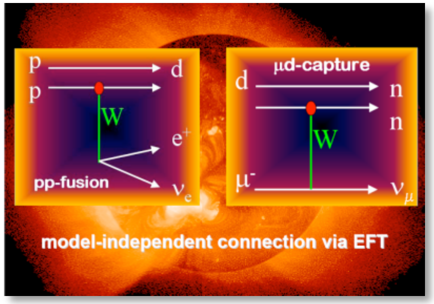
(**Moridis , LBNL, *Water Resources Research)***



Nuclear Physics

Scientists use Edison to perform the first LQCD calculations of the radiative capture process.

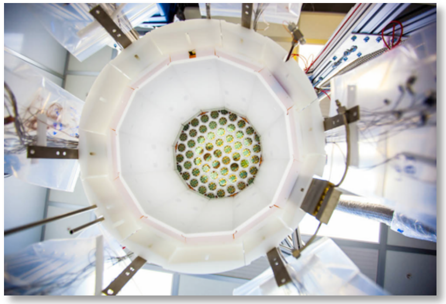
(Savage, U. Washington, *Phys. Rev. Lett.)*



High Energy Physics

New tools handle increasingly large datasets produced by ATLAS experiments at the Large Hadron Collider.

(LeCompte, ANL; Hinchliffe, Berkeley Lab, Journal of Physics Conf. Series)



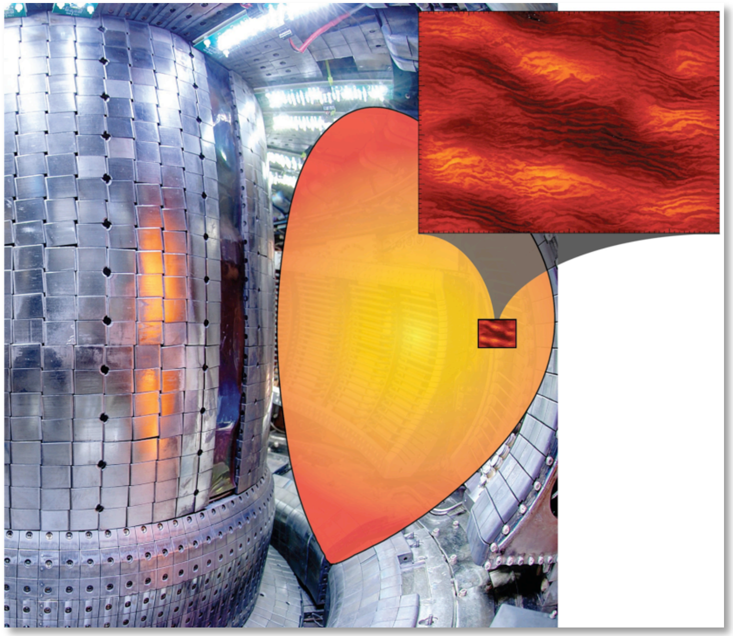
Solving a Plasma Turbulence Mystery

Scientific Achievement

A series of simulations run on Edison found that interactions between turbulence at the tiniest scale (electrons) and turbulence at a scale 60 times larger (ions) accounts for the mismatch between theoretical predictions and experimental observations of heat loss in tokamak fusion reactors.

Significance and Impact

This research has yielded answers to long-standing questions about plasma heat loss that have previously stymied efforts to predict the performance of fusion reactors and could help pave the way for this alternative energy source.



The inside of the Alcator C-Mod tokamak, with a representative cross-section of a plasma. The inset shows the approximate domain for one of the multi-scale simulations and the plasma turbulence in the multi-scale simulation.
Image: Nathan Howard.

Research Details

- 2D and 3D simulations were run at NERSC over a two-year period.
- By performing high-resolution multi-scale simulations, the team simultaneously modeled multiple turbulence instabilities that have previously been treated in separate simulations.
- The study took between 100 million and 120 million core hours on Edison. Each simulation required about 15 million hours of computation running on 17,000-30,000 processors

Howard, Holland, White, Greenwald and Candy, Nuclear Fusion, Vol. 56, No. 1, Dec. 17, 2015

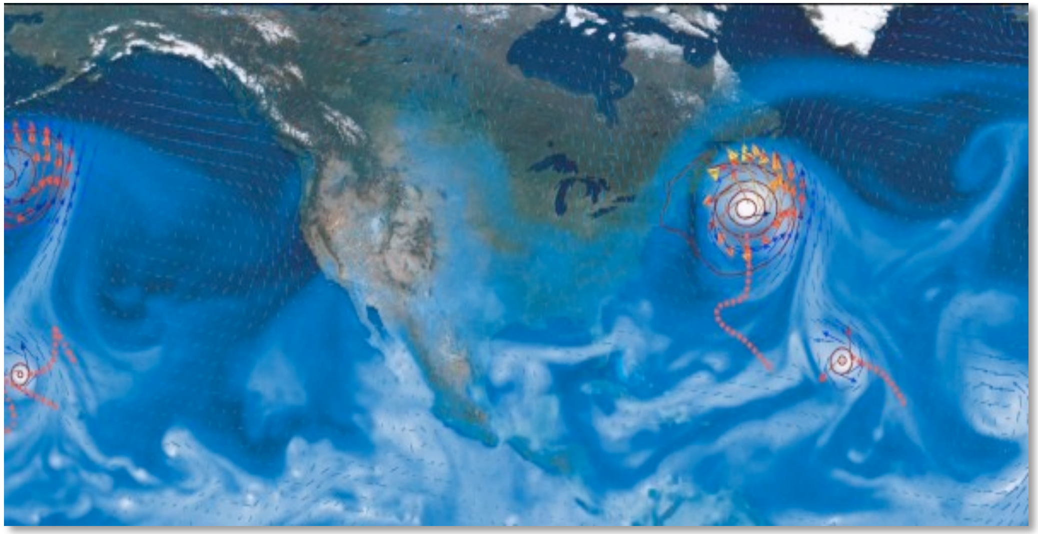
Tracking Extreme Weather in Climate Simulations

Scientific Achievement

Using new advanced software named TECA running at NERSC, researchers have reduced the time needed to detect important features in large climate datasets from years to hours.

Significance and Impact

Climate simulations produce massive amounts of data, requiring sophisticated pattern recognition algorithms to identify significant weather events. The Toolkit for Extreme Climate Analysis (TECA) was developed at Berkeley Lab to address this need.



TECA implements multi-variate threshold conditions to detect and track extreme weather events in large climate datasets. This visualization depicts tropical cyclone tracks overlaid on atmospheric flow patterns.

Research Details

- A team from Berkeley Lab and Argonne used TECA on NERSC's Hopper and Argonne's Mira systems to analyze 56 TB of climate data from the 5th phase of the Coupled Model Intercomparison Project to identify 3 classes of storms: tropical cyclones, atmospheric rivers and extra-tropical cyclones.
- NERSC's Hopper 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 in Sept. 2015, was awarded the Juelich Supercomputing Center prize for the best application of HPC technology in solving a pattern recognition problem

D. Millstein, R. Levinson, P. Rosado, M. Cao, Z. Lin, *Environmental Science & Technology,* November 2015, 49, 14672-14679

Assessing the Impact of 'Fracking' on Groundwater

Scientific Achievement

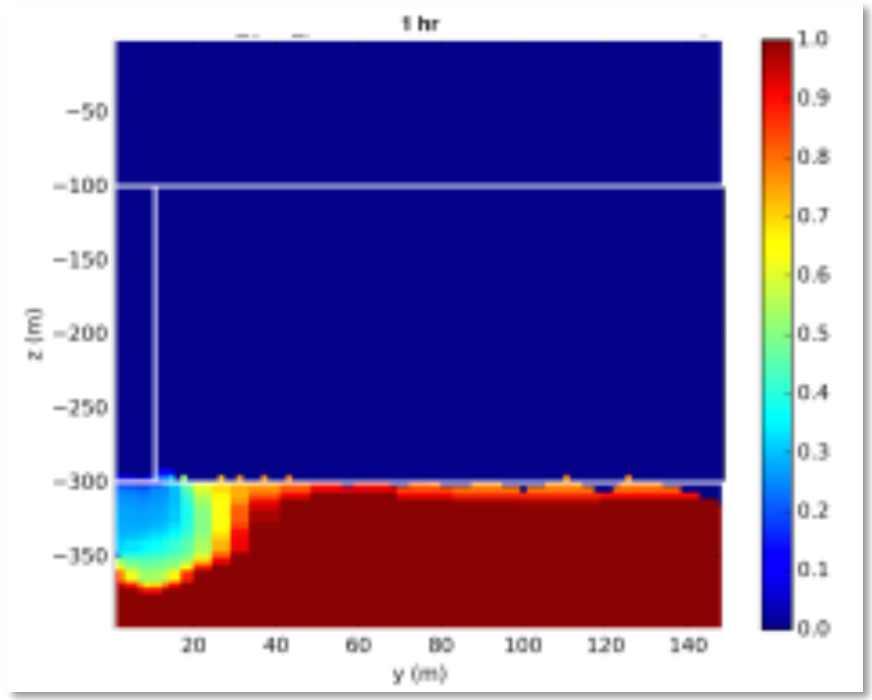
Using NERSC supercomputers, researchers have found that, except for a brief period following fracking operations, water flow is uniformly downward, away from the fresh-water aquifer.

Significance and Impact

These findings support a 2015 EPA study that concluded below-ground migration of liquids and gases due to fracking have not had widespread impact on U.S. drinking water resources.

Research Details

- The numerical simulations, run on NERSC's Hopper and Edison systems, evaluated the transport of contaminants (initially gas) from a tight-sand and shale gas reservoir to a shallower aquifer.
- The researchers found that, except for a brief initial period of upward flow during the initial phase of rapid gas ascent in the connecting feature, water flow is uniformly downward.



Gas phase saturation (S_G) in the plane of the connecting fracture at t = 1.0 hour.

M. Reagan, G. Moridis, N. Keen, J. Johnson
Water Resources Research, Volume 51, Issue 4, April 2015, 2543–2573

First LQCD Calculation of Inelastic Nuclear Reaction

Scientific Achievement

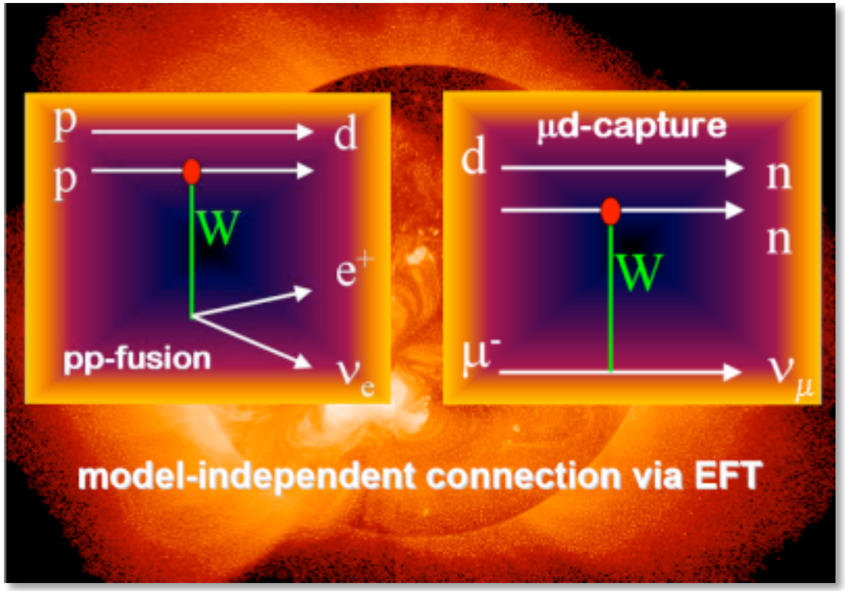
Scientists used NERSC's Edison system to perform the first lattice quantum chromodynamics (LQCD) calculations of the process whereby a neutron and proton combine to form a deuteron, the nucleus of "heavy" hydrogen.

Significance and Impact

Understanding this "radiative capture" process and the precise determination of the rate at which it occurs are critical to understanding big bang nucleosynthesis, fusion in the sun, and solar neutrino oscillations. These results are the first to be derived directly from the fundamental theory of the strong nuclear force, QCD.

Research Details

- LQCD calculations were used to determine the short-distance two-nucleon interactions with the electro-magnetic field that significantly contribute to the low-energy cross sections for the radiative capture process.
- This work reinforces the utility of combining LQCD calculations with low-energy effective field theories describing multinucleon systems.



The MUSUN experiment at the University of Washington is measuring the rate for muon capture on the deuteron to better than 1.5% precision. This process is the simplest weak interaction process on a nucleus that can both be calculated and measured to a high degree of precision.

S. Beane, E. Chang, W. Detmold, K. Orginos, A. Parreno. M. Savage, B Tiburzi
Physical Review Letters, 115, 132001
September 24, 2015

Updated Workflows Enhance New LHC Era

Scientific Achievement

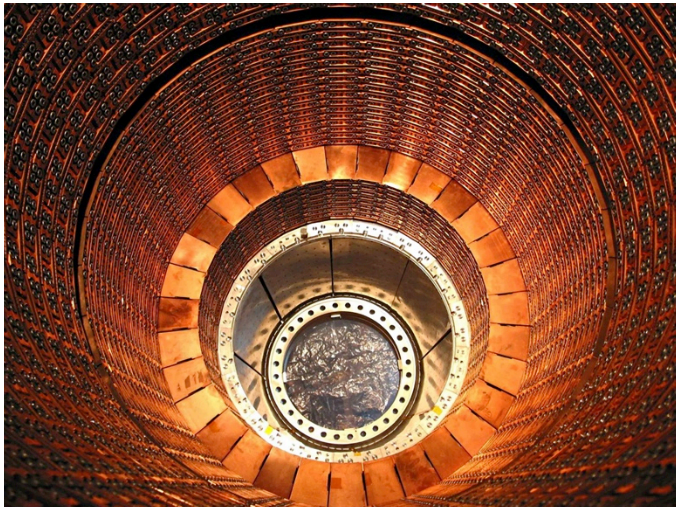
Two new workflow management tools developed at LBNL to handle increasingly large datasets produced by ATLAS experiments at the Large Hadron Collider—the world's most powerful particle collider—are helping physicists maximize next-generation supercomputing architectures

Significance and Impact

After a massive upgrade, the LHC is now capable of producing up to 1 billion collisions and generating up to 10 gigabytes of data; the new tools make reconstruction, simulation and data analysis more efficient

Research Details

- To deal with this "data deluge," LBNL researchers developed Yoda and AthenaMP and tested them on NERSC's Edison supercomputer.
- Yoda replicates the LHC Computing Grid workflow on a supercomputer, while AthenaMP allows the ATLAS reconstruction, simulation and data analysis framework to run efficiently on massively parallel systems.
- The team tested Yoda's performance by running ATLAS jobs from the previous LHC run on Edison and successfully scaled up to 50,000 cores.



A view inside the LHC's liquid-argon calorimeter endcap. Image: The ATLAS Experiment at CERN

P. Calafiura, et al, on behalf of the ATLAS Collaboration, *Journal of Physics: Conference Series* 664, (2015) 092025

PIs: I. Hinchliffe (Berkeley Lab), T. LeCompte (Argonne)

National Energy Research Scientific Computing Center