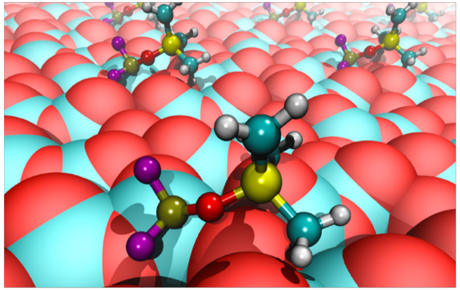
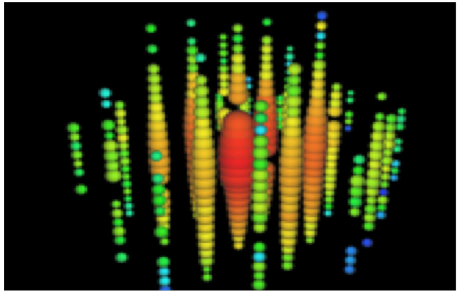
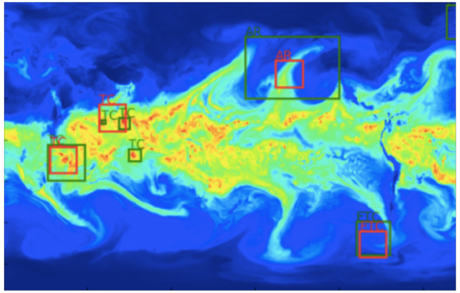
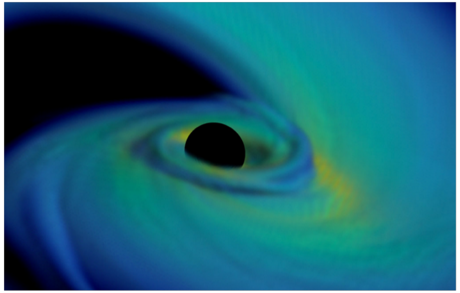
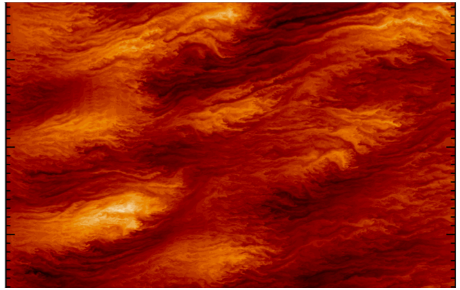
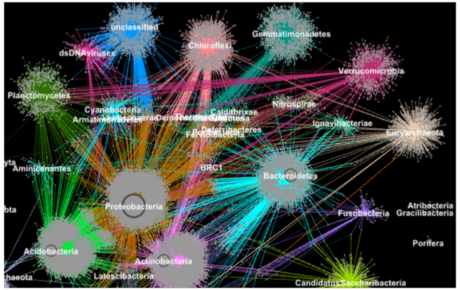
NERSC Science Highlights

June 2018

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NERSC Science Highlights

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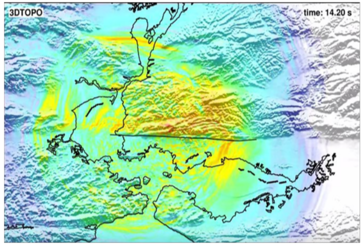
Earth Systems

Quantifying Earthquake Hazard and Risk

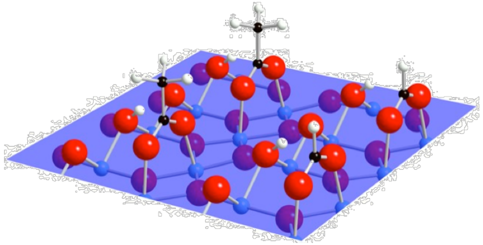
NERSC PI: McCallen, Berkeley Lab, 11th National Conference on Earthquake Engineering

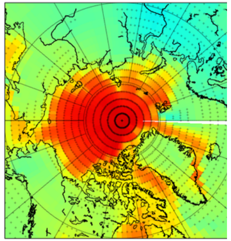


Materials Science

Unraveling the Mysteries of Self-Cleaning TiO_2

NERSC PI: Hines, Cornell University. *Science*

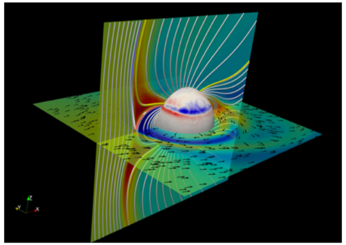




Earth Science

Resolving an Artic Modeling Puzzle

NERSC PI: Feldman, Berkeley Lab. *Journal of Geophysical Research*



Plasma Physics

Understanding Auroras on Ganymede

NERSC PI: Bhattacharjee, Princeton, National Lab. *Journal of Geophysical Research*

High Energy Physics

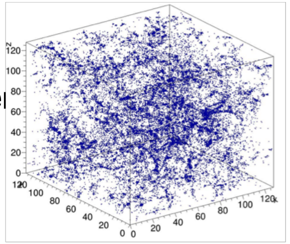
Evidence of Antineutrino Oscillation

NERSC Pis: Gutsche, Kowalkowski, Fermilab. *Neutrino 2018*

Cosmology

Determining Cosmological Parameters with Deep Learning

NERSC PI: Bard, Berkeley Lab. *SC18*



Quantification of Earthquake Hazard and Risk

Scientific Achievement

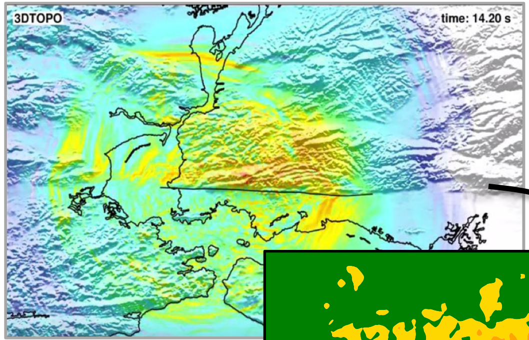
Researchers from Berkeley Lab and Livermore Lab used the large scale of NERSC's Cori supercomputer to simulate the impact of a major earthquake at unprecedented resolution. The models predict how it would affect different buildings in the Bay Area depending on building location and size.

Significance and Impact

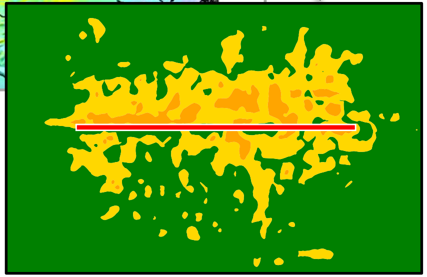
Historically, seismic experts have used empirical evidence from previous earthquakes to assess regional hazard and risk. While data about ground motion characteristics and resulting structural damage from an earthquake that occurred halfway across the world can help, it can't adequately inform our understanding of how well infrastructure in California or other quake prone regions of the U.S. would be affected. The new simulations allow unprecedented, high-fidelity, site-specific risk assessments of infrastructure risk at regional scale.

Research Details

Working closely with experts in systems, data, and applications from NERSC, the researchers used essentially the entire Cori machine to simulate ground shaking seismic waves at 5 cycles per second (5 Hz) over the entire San Francisco Bay Area region for a magnitude 7 earthquake on the Hayward Fault. The run took over 9 hours to complete, using 8,192 nodes (524,288 compute cores). The team took advantage of Cori's unique flash burst-buffer file system for massive I/O to save their large data sets quickly.



Simulated ground motions for a M=7 earthquake



Corresponding damage for 3 story steel frame buildings

Images resulting from simulations run at NERSC show the distribution of ground motion intensity and resulting structural risk across the San Francisco Bay Area region after a large-magnitude earthquake along the Hayward Fault. Credit: David McCallen

3 papers summarizing this work were presented at the 11th National Conference on Earthquake Engineering in June 2018

Unraveling the Mysteries of Self-Cleaning TiO_2

Scientific Achievement

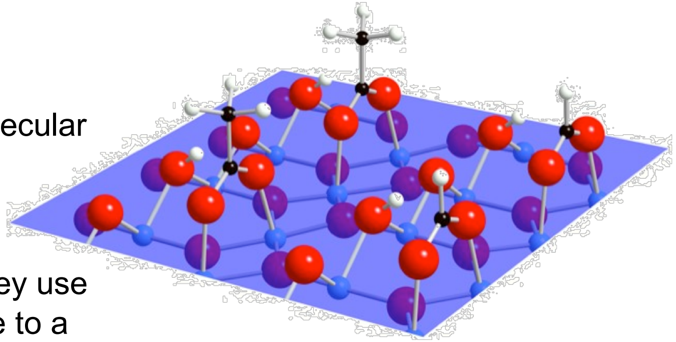
Simulations run at NERSC helped researchers from Cornell University and Technical University of Vienna, Austria, begin to decipher how ordered molecular structures form on the surface of Titanium Dioxide (TiO_2).

Significance and Impact

Titanium dioxide (TiO_2) is one of several minerals that are self-cleaning; they use energy from the sun to convert any dirt or debris that lands on their surface to a harmless gas, which then floats away. These minerals have been used in self-cleaning glass and in cements, tiles, and paints to help maintain clean surfaces. But how this worked at the molecular level was not known. A more detailed understanding of the surface chemistry will pave the way for further commercialization of products useful for environmental remediation and self-sterilizing construction materials.

Research Details

The researchers ran a series of density functional theory simulations of TiO_2 surfaces and their chemistry at NERSC. Comparing these simulations to scanning tunneling microscopy images and surface vibrational spectroscopy experiments, the researchers found that when TiO_2 is exposed to air, the surface becomes covered with a single-molecule-thick layer of two organic acids: acetic acid (vinegar) and its close relative, formic acid.



Density functional theory simulation of a formate/acetate monolayer.

NERSC HPC Consultant Zhengji Zhao provided support and assistance to the team with their materials science code.

J. Balajka, et al, Science, August 2018, Vol. 361, Issue 6404, doi: 10.1126/science.aat6752

Resolving an Artic Modeling Puzzle

Scientific Achievement

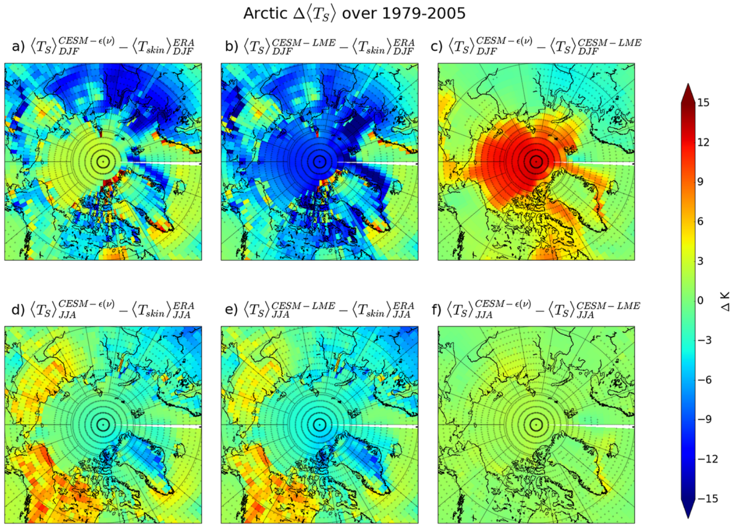
A team led by Berkeley Lab researchers included a novel feedback mechanism from unfrozen surfaces in the Artic to help explain why climate models have consistently underestimated the temperature and magnitude of climate change at high latitudes

Significance and Impact

It is important that climate models can correctly reproduce observations. The IPCC Fifth Assessment Report found that the average surface air temperatures across the poles were significantly colder in models than observed. This implies an underestimation of high-latitude warming by current climate models, which has profound implications both for the far north as well as lower latitudes. By including a new model of how ice radiates back into the atmosphere, the authors found that the discrepancy between models and measurements disappeared in their climate model.

Research Details

The team used Cori, Edison, the NERSC global file system, and the HPSS archival storage system to run their simulations and store data. NERSC's Jupyter notebook service was "extremely helpful" with their analysis.



Time-Dependent Cryospheric Longwave Surface Emissivity Feedback in the Community Earth System Model, Volume: 123, Issue: 2, Pages: 789-813, First published: 03 January 2018, DOI: (10.1002/2017JD027595)

Kuo, Chaincy; Feldman, Daniel R.; Huang, Xianglei; Flanner, Mark; Yang, Ping; Chen, Xiuhong, "JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES, 123:789-813; 2018 JAN 27, 10.1002/2017JD027595

Understanding Auroras on Ganymede

Scientific Achievement

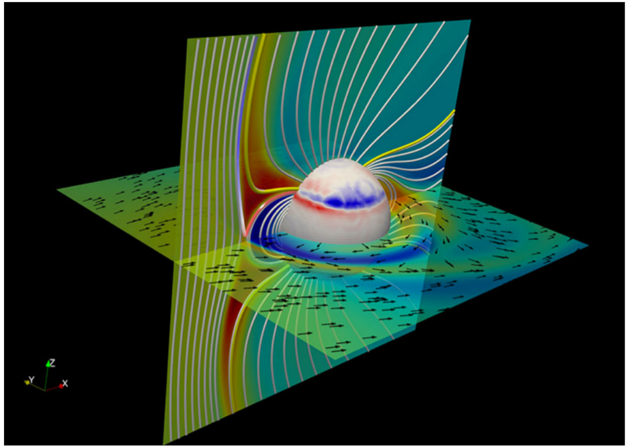
Using supercomputer simulations run at NERSC covering the entire magnetosphere of Jupiter's moon Ganymede, researchers revealed how electrons from Jupiter's atmosphere are accelerated and collide with Ganymede's polar regions.

Significance and Impact

Ganymede is the only moon in the solar system that displays auroras, which yield important information about space weather. Comparing simulations with observations produces crucial clues about how auroras form on Earth and other planets. The research also helps researchers understand if solar flares will knock out satellites.

Research Details

The simulations included oxygen ions and electrons and self-consistently compute their density, momentum, and pressure. The model correctly captured key features of Ganymede's magnetosphere, such as the wing-like structure and the variations in the brightness of Ganymede's surface (deducible from the oxygen ions and electrons pressure, shown in figure).



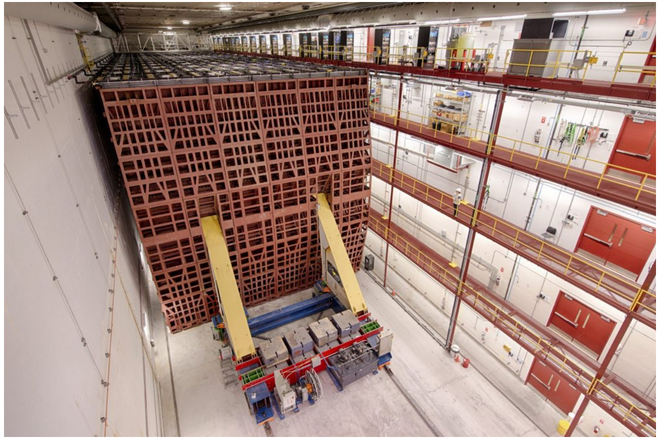
The global structure of the magnetosphere of Ganymede is revealed by 3-D two-fluid modeling. Regions of high and low pressure are shown in red and blue in the equatorial and meridional planes. Image: Liang Wang, Princeton Univ.

L. Wang, et al, Journal of Geophysical Research: Space Physics 123, 2815 (2018), doi: 10.1002/2017JA024761

Evidence of Antineutrino Oscillation

Scientific Achievement

The NOvA neutrino experiment, in collaboration with the Department of Energy's Scientific Discovery through Advanced Computing (SciDAC-4) program and the HEPCloud program at DOE's Fermi National Accelerator Laboratory (Fermilab), was able to perform the largest-scale analysis ever to support the recent evidence of muon antineutrinos oscillating into electron antineutrinos over long distances, a phenomenon that has never been unambiguously observed.



Fermilab's NOvA neutrino experiment announced that it had seen strong evidence of muon antineutrinos oscillating into electron antineutrinos over long distances. Photo: Reidar Hahn

Significance and Impact

Precisely measuring how neutrinos and antineutrinos change from one type into another, and then comparing them, will help scientists unlock the secrets that these particles hold about how the universe operates.

Research Details

Using NERSC's Cori and Edison supercomputers, NOvA used nearly 35 million core-hours in a 54-hour period. This unprecedented amount of computing enabled scientists to do analysis of real data coming off the detector at a rate 50 times faster than that achieved in the past. The first round of analysis was done within 16 hours. Experimenters were able to see what was coming out of the data, and in less than six hours the entire collaboration was looking at it.

Results were presented at Neutrino 2018 conference

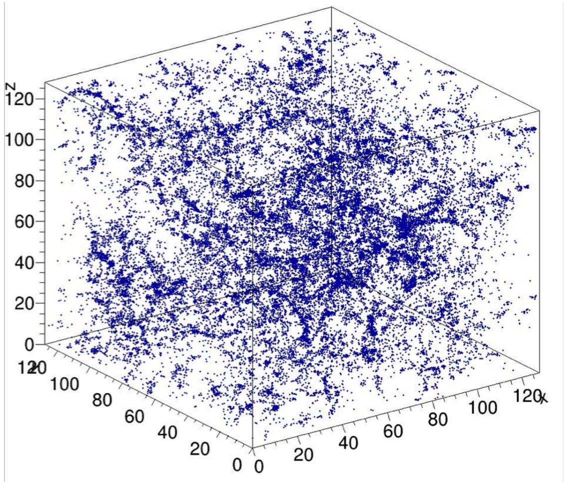
Determining Cosmological Parameters with Deep Learning

Scientific Achievement

Data scientists from NERSC/Berkeley Lab, UC Berkeley, Cray, and Intel ran the first large-scale science application of the TensorFlow framework at supercomputer scale with fully-synchronous training to predict the cosmological parameters Ω_m, σ_8 and N_s from the dark matter distribution in the universe with unprecedented accuracy.

Significance and Impact

The distribution of matter at the largest scales tells us about the fundamental physics of universe involving gravity, dark matter, and dark energy. The three parameters Ω_m, σ_8 and N_s describe the fraction of matter in the universe, the size of mass fluctuations and the curvature of space-time. Scientists want to extract the underlying physics from the structure and Deep Learning techniques offer a way to determine these parameters from observations.



Example simulation of dark matter in the universe, used as input to the CosmoFlow network.

Research Details

- The team used the results from cosmological simulations to train the algorithms to recognize signatures of the differing parameters used to create the simulations.
- The training dataset was 1.4 TB, scaled up from previous work using a 62 GB set.
- An optimized version of TensorFlow was run on Cori, which achieved 77% scaling efficiency on 8,192 Intel Xeon Phi nodes and 3.5 petaflops of total performance.

Bard, D.; Mathuriya, A.; et al., CosmoFlow: *Using Deep Learning to Learn the Universe* was presented at SC18.

NERSC PI: Deborah Bard, Berkeley Lab

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