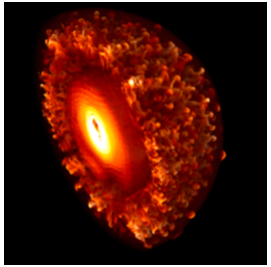
Science Highlights

Nuclear Astrophysics

World's first 3-D Simulations of Superluminous Supernovae

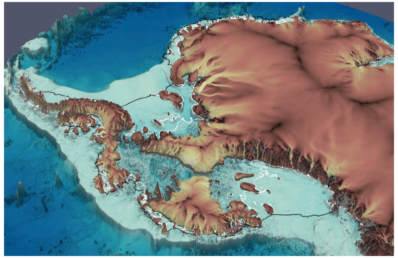
NERSC PI: Ken Chen. Academia Sinica Taiwan, UC Santa Cruz. *Astrophysical Journal*

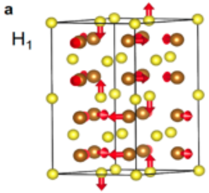


Environment

New Estimates for Ice Sheet Mass Loss

NERSC PI: Stephen Price, Los Alamos National Laboratory. *Cryosphere.*





Materials Science

Designing Materials with Tunable Electrical and Magnetic Behaviors

NERSC PI: Oliver Delaire, Duke University. *Nature Physics*

Fusion Energy

Near-Real Time Networked Analysis of Big KSTAR Data

NERSC PI: C.S. Chang, Princeton Plasma Physics Lab. *Physics of Plasmas*

COVID Scholar

COVID Response

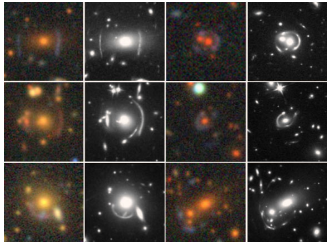
Machine Learning Tool Could Provide Unexpected Scientific Insights

NERSC PI: Kristin Persson, Lawrence Berkeley National Laboratory. *https://covidscholar.org*

Cosmology

Discovering Hundreds of New Gravitational Lenses

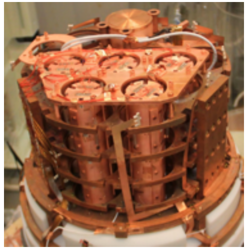
NERSC PI: David Schlegel, Berkeley Lab. *Astrophysical Journal*



Nuclear Physics

Searching for Evidence of a 'Neutrinoless' Particle Process

NERSC PI: Yury Kolomensky, Berkeley Lab. *Neutrino 2020*



World's first 3-D Simulations of Superluminous Supernovae

NERSC

Scientific Achievement

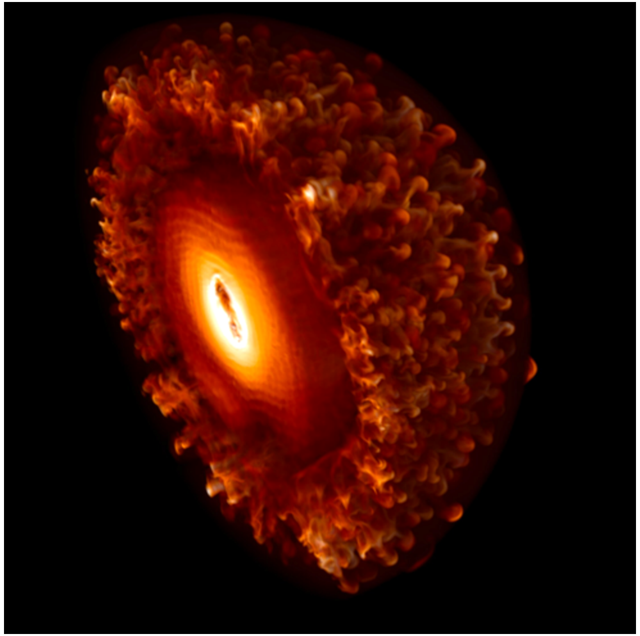
For the first time ever, an international team of astrophysicists simulated the three-dimensional (3-D) physics of superluminous supernovae — which are about a hundred times more luminous than typical supernovae. They achieved this milestone using Berkeley Lab's CASTRO code and supercomputers at NERSC.

Significance and Impact

Superluminous supernovae are perhaps the brightest explosions in the universe, but the physics behind these events is not well understood. These new simulations reveal that additional instabilities, not present in ordinary supernovae, occur that help drive the explosion. Their simulations also explain certain observations, like why iron is observed early in core-collapse supernovae events like SN 1987A. This has been a long-standing mystery in astrophysics.

Research Details

The team needed NERSC supercomputers to model the required physics over many scales and in 3 dimensions. Lower dimensional models can not capture all the important effects, such as fluid instabilities The observed instabilities drive mixing within the system, which affects how quickly the supernovas brighten and dim and what elements are observed in their spectra.



The nebula phase of the magnetar-powered super-luminous supernova from the team's 3D simulation. The supernova ejecta has expanded to a size similar to the solar system. Large scale mixing appears at the outer and inner region of ejecta. The resulting light curves and spectra are sensitive to the mixing that depends on stellar structure and the physical properties of magnetar. Credit: Ken Chen

NERSC PI: Ken Chen, Academia Sinica Taiwan; Compute Award from DOE Office of Nuclear Physics; Funding from the National Science Foundation

Ken Chen received the NERSC 2015 High Impact Scientific Achievement Early Career Award while a post-doctoral researcher at UC Santa Cruz.

Chen, Woosley and Whalen, Astrophysical Journal, 893:99, 2020 April 20 https://doi.org/10.3847/1538-4357/ab7db0

New Estimates for Ice Sheet Mass Loss

Scientific Achievement

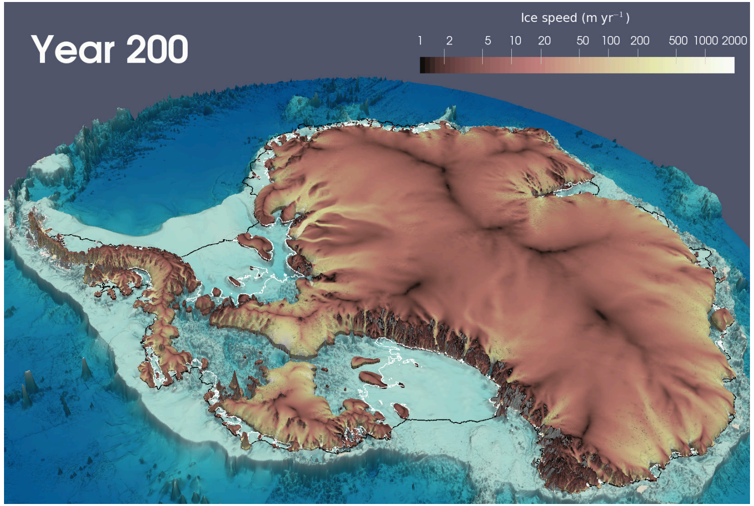
An international consortium of researchers has calculated new estimates for the melting of Earth's ice sheets due to greenhouse gas emissions and its impact on sea levels, showing that ice sheets could contribute more than 40 cm of rise by 2100.

Significance and Impact

As sea levels continue to rise due to increased melting and retreat of the Greenland and Antarctic ice sheets, large areas of densely populated coastal land will be affected. It is important to understand the impact climate change could have on the rate of melting and, consequently, changes in sea level.

Research Details

- The Ice Sheet Model Intercomparison Project for CMIP6 (ISMIP6), consisting of more than 60 scientists from 36 institutions across the world, used the latest generation of climate and ice sheet models to estimate the impacts of a changing climate on ice sheets and sea level.
- Results were presented under multiple publications in a special issue of the journal *The Cryosphere,* published between June and October of 2020.
- A team led by Stephen Price and Esmond Ng used the Los Alamos, Sandia, and Berkeley Lab-developed MALI and BISICLES ice sheet models for the study.
- All ISMIP6 simulations conducted by DOE were run on NERSC supercomputers.



Antarctic ice sheet 200 years after all floating ice shelves are removed. Shown are simulation results from ProSPect MALI

NERSC PIs: Stephen Price, Los Alamos National Laboratory; Compute Award and funding from DOE Office of Biological and Environmental Science; Esmond Ng, Lawrence Berkeley National Laboratory, Compute Award and funding from the DOE Office of Advanced Scientific Computing Research

Special Issue: The Ice Sheet Model Intercomparison Project for CMIP6 (ISMIP6). *The Cryosphere*, https://tc.copernicus.org/articles/special_issue1019.html

Designing Materials with Tunable Electrical and Magnetic Behaviors

Scientific Achievement

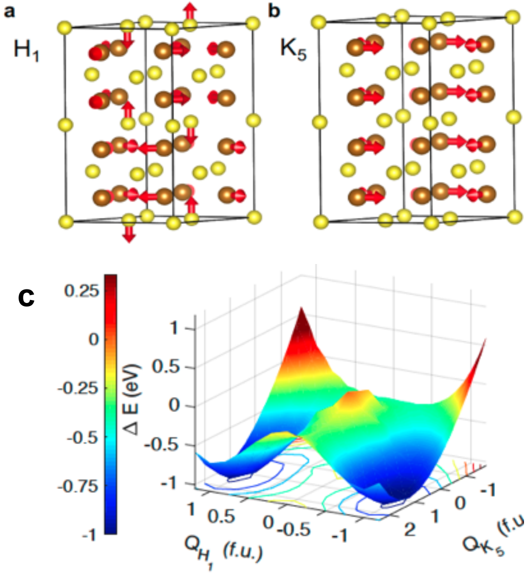
For the first time, the coupling of magnetic spins and atomic dynamics has been fully described in hexagonal iron sulfide (*h*-FeS), explaining the origin of its metal-insulator transition.

Significance and Impact

This discovery provides a new route to design materials with tunable electrical and magnetic behaviors for possible applications in information storage and processing.

Research Details

- The team used inelastic neutron scattering and inelastic x-ray scattering along with first-principles simulations to track evolution of the lattice and spin dynamics across the magnetic and metal-insulator transitions.
- Research establishes that the ordering of magnetic spins on Fe atoms destabilizes the vibrations of atoms (H_1 and K_5 modes in figure), and leads to a structural distortion opening the band gap (insulator phase).
- Strongly anharmonic lattice vibrations associated with unstable phonon modes are controlled by magnetic ordering of spins and in turn provide the structural distortion tuning the band-gap. Thus, spin-phonon and electron-phonon couplings are key to enable the sequence of phase transitions in *h*-FeS.
- The work used HERIX spectrometer at APS sector 30 (ANL), ARCS & SEQUOIA spectrometers at the SNS (ORNL), and about 1 million hours on 512 concurrent CPU cores at NERSC.



Lattice instabilities enabled by antiferromagnetic ordering in h-FeS.

D. Bansal, J. L. Niedziela, S. Calder, T. Lanigan-Atkins, R. Rawl, A. H. Said, D. L. Abernathy, A. I. Kolesnikov, H. Zhou, and O. Delaire, Nature Physics, (2020).
DOI: https://doi.org/10.1038/s41567-020-0857-1.

NERSC PI: Oliver Delaire, Duke University; Compute Award and funding from DOE Office of Basic Energy Sciences

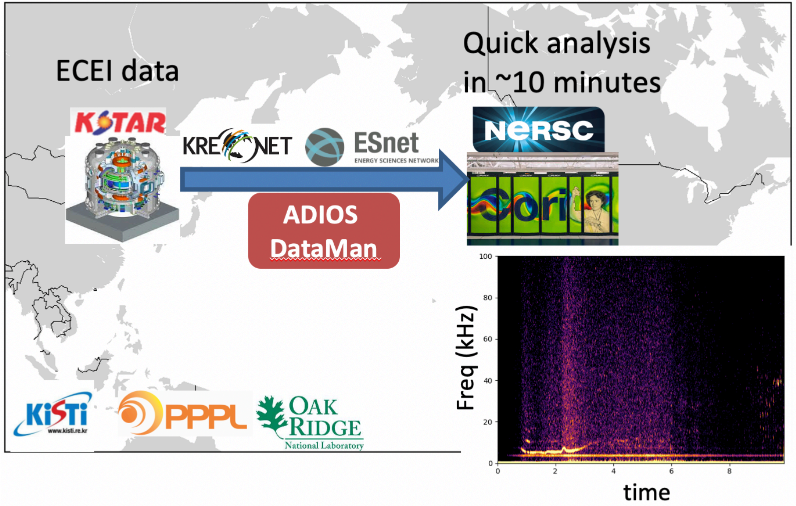
Near-Real Time Networked Analysis of KSTAR Data

Scientific Achievement

Scientists and engineers have established a near real-time networked analysis of data taken at the KSTAR fusion experiment in South Korea. The framework is using Machine Learning and Artificial Intelligence algorithms running at NERSC for analysis of large data streams.

Significance and Impact

Fusion reactors have the potential to provide a huge source of clean and affordable electricity. Experiments are underway around the world to turn this promise into reality. These new capabilities allow United States fusion researchers to have broader and faster access to KSTAR (and future ITER) data, enabling faster analysis and informed steering of the fusion experiments.



Research Details

- The end-to-end Python framework DELTA streams data using ADIOS DataMan over WAN (at rates > 4 Gbps), asynchronously processes on multiple workers with MPI & multi-threading
- Implemented deep convolutional neural networks for working with multi-scale fusion data, e.g. ECEi, for recognizing events of interest.
- With KSTAR data streaming to NERSC, the time for an ECEi analysis was reduced from 12 hours on single-process to 10 minutes on 6 Cori nodes.

R. Kube, RM Churchill, J. Choi, et al., SciPY 2020 Conference Proceedings, "Leading magnetic fusion energy science into the big-and-fast data lane," http://doi.org/10.25080/Majora-342d178e-013 .

NERSC PI: C.S. Chang, Princeton Plasma Physics Laboratory; Compute Award and funding from DOE Office of Fusion Energy Sciences

Discovering Hundreds of New Gravitational Lenses

Scientific Achievement

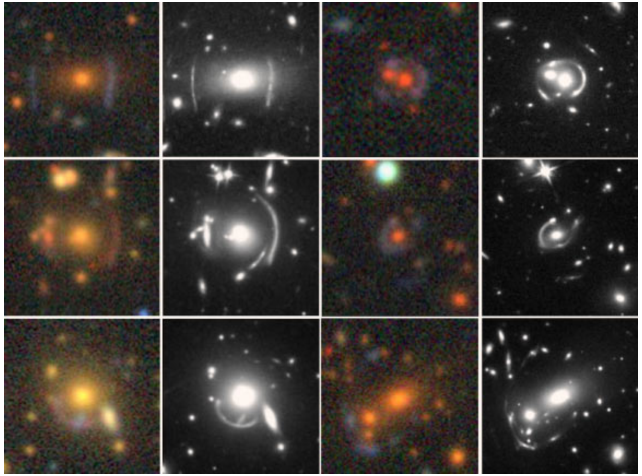
Scientists used neural networks running on Cori to identify 335 new gravitational lens candidates from data collected for in the Dark Energy Camera Legacy Survey (DECaLS) .

Significance and Impact

Gravitational lensing occurs when a large mass bends light, according to the laws of Einstein's General Relativity, from a background object. The images of lensed objects appear to observers on Earth as circles, arcs, and other distortions. Those shapes help scientists measure distances to galaxies, map the mass distribution of the universe, and investigate the nature of dark energy.

Research Details

- The lens candidates were identified with the assistance of a neural network, which is a form of artificial intelligence in which the computer program is trained to gradually improve its image-matching over time to provide an increasing success rate in identifying lenses.
- The team used the Shifter container technology developed at NERSC to run the "Tractor" software that applies neural networks to identify new candidates based on a training set of known lenses.
- DECaLS is one of the Dark Energy Spectroscopic Instrument (DESI) Legacy Imaging Surveys, conducted in preparation for the upcoming DESI survey.



Sde-by-side comparisons of gravitational lens candidates imaged by DECaLS (color) and the NASA/ESA Hubble Space Telescope (B&W). Image credit: DECaLs/ NASA / ESA / Hubble / Huang et al.

Huang, et al., "Finding Strong Gravitational Lenses in the DESI DECam Legacy Survey"; ASTROPHYSICAL JOURNAL, 894 2020 MAY, 10.3847/1538-4357/ab7ffb

NERSC PI: David Schlegel, Berkeley Lab; Compute Award and funding from DOE Office of High Energy Physics; Additional compute award from the NERSC High Impact Science Director's Reserve program

NERSC Plays Key Role in CUPID-Mo Collaboration

Searching for Evidence of a 'Neutrinoless' Particle Process

Scientific Achievement

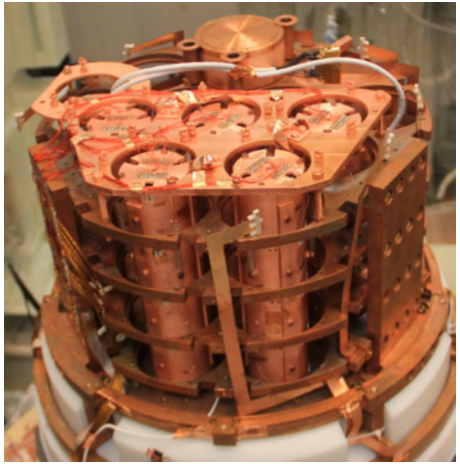
Nuclear physicists at Berkeley Lab played a leading role in analyzing data for a demonstration that achieved record experimental precision using a specialized detector material. The data analysis component of this ground-breaking research was conducted entirely at NERSC.

Significance and Impact

The CUPID-Mo experiment is among a field of experiments using a variety of approaches to detect a theorized particle process, called neutrinoless double-beta decay, that could revise our understanding of ghostly particles called neutrinos, and of their role in the evolution of the universe. Preliminary results from CUPID-Mo, based on analysis of data collected from March 2019 to April 2020, set a new world-leading limit for the neutrinoless double-beta decay process in an isotope of molybdenum known as Mo-100

Research Details

- All of the data from the CUPID-Mo experiment – the CUPID acronym stands for CUORE Upgrade with Particle IDentification, and "Mo" is for the molybdenum contained in the detector crystal – is transmitted from the Modane Underground Laboratory in France to the Cori supercomputer at NERSC.
- The availability and reliability of Cori during the work-from-home restrictions around the world were key to preparing the results in time for the Neutrino2020 conference in June 2020.
- Benjamin Schmidt, a postdoctoral researcher in Berkeley Lab's Nuclear Science Division, led the overall data analysis effort for the CUPID-Mo result.



The CUPID-Mo detector is installed in the Edelweiss cryostat at Modane Underground Laboratory (LSM) in France. (Credit: CUPID-Mo collaboration)

T. O'Donnell, Neutrino 2020 Conference, 10.5281/zenodo.3959650

NERSC PI: Yury Kolomensky, Berkeley Lab; Compute Award and funding from DOE Office of Nuclear Physics

Machine Learning Tool Could Provide Unexpected Scientific Insights into COVID-19

COVID Scholar

https://covidscholar.org

Scientific Achievement

Working closely with NERSC, a team of materials scientists at Berkeley Lab have created a text-mining tool in record time to help the global scientific community synthesize the mountain of scientific literature on COVID-19 being generated every day.

Significance and Impact

COVID Scholar uses natural language processing techniques to quickly scan and search tens of thousands of research papers and draw insights and connections that may otherwise not be apparent. COVID Scholar was developed in response to a call to action from the White House Office of Science and Technology Policy that asked AI experts to develop new data and text mining techniques to help find answers to key questions about COVID-19. COVID Scholar is also being used by MIT's Rapid Review Journal, the KG-COVID knowledge graph project and in Pacific Northwest National Lab's literature analysis tool.

Research Details

Assisted by quick access to NERSC's Cori supercomputer, the center's "Spin" internal cloud for edge services, and expert staff assistance from NERSC staff, a prototype was created in just 7 days. State of the art natural language processing models run daily on Cori and the search portal is running on the NERSC "Spin" edge services cluster.

Berkeley Lab researchers (clockwise from top left) Kristin Persson, John Dagdelen, Gerbrand Ceder, and Amalie Trewartha led development of COVIDScholar. (Credit: Berkeley Lab)

NERSC PI: John Dagdelen, Berkeley Lab; Compute Award from NERSC Director's Discretionary Reserve; Funding from the Energy Biosciences Institute at UC Berkeley, the National Science Foundation, and the C3.ai Digital Transformation Institute.