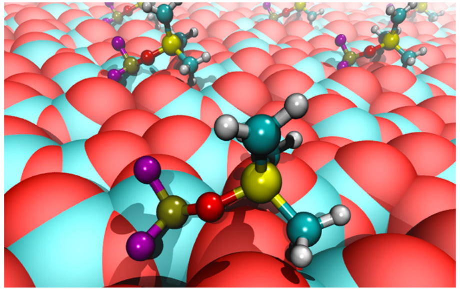
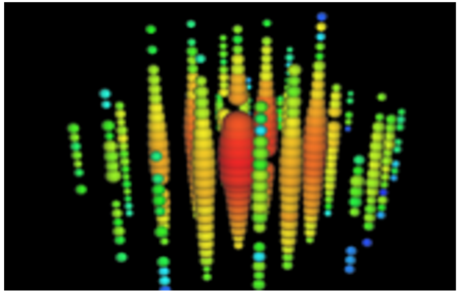
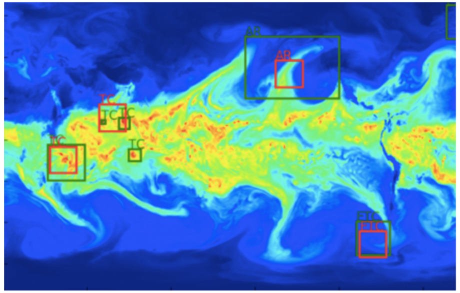
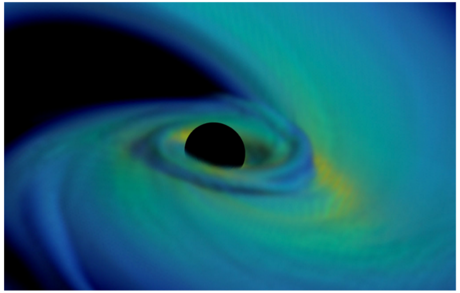
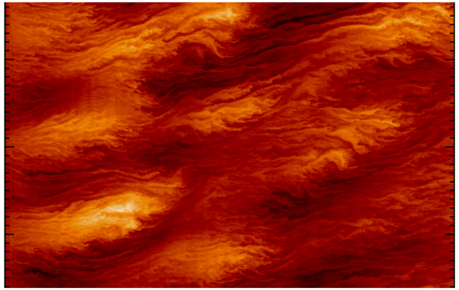
NERSC Science Highlights

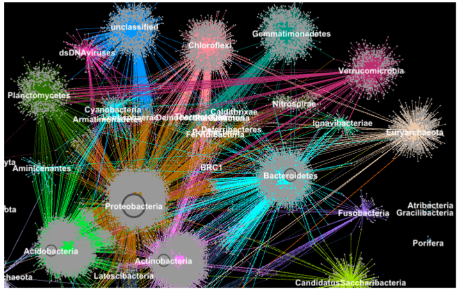










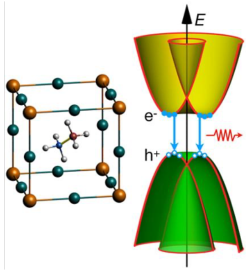


NERSC

Science Highlights

Revealing Mechanisms for Solar Cells

Researchers from UC Santa Barbara are better understanding the solar conversion efficiencies of hybrid perovskites and gaining critical insights into how they work.



Constraints on the Size of Neutron Stars

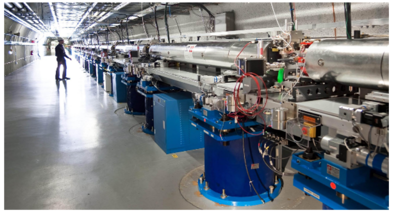
Scientists have determined with unprecedented accuracy that a neutron star with 1.4 times the mass of our Sun is packed into a sphere 11.75 km in radius.

Urban Landscapes Boost Destructive Storms

A team from Pacific NW Lab found that urban landscapes and pollution can make wind gusts stronger, rain heavier, hail larger and even steer storms toward cities.

Energy Storage

Scientists from UC San Diego developed a new material that makes batteries safer, holds more charge and charges faster.

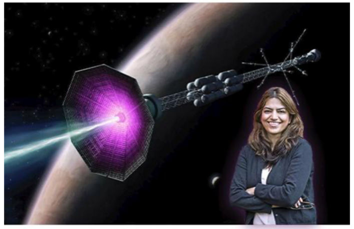


NERSC & LCLS Team Up on COVID Research

The collaboration allowed scientists to study the SARS-CoV-2 virus in unprecedented detail.

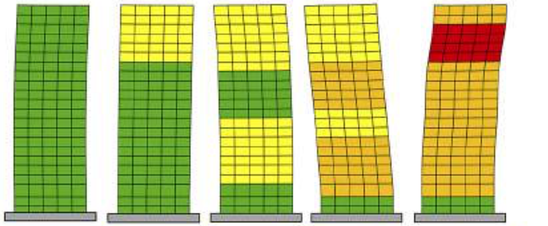
Rocket Thruster Could Propel Humans to Mars and Beyond

The proposed device can generate exhaust with velocities of hundreds of kilometers per second.



Regional Simulations of Building Response to Major Earthquakes

The study looked at many scenarios of interest to inform civic planners so they can save lives and protect infrastructure.



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Revealing Reclusive Mechanisms for Solar Cells

Scientific Achievement

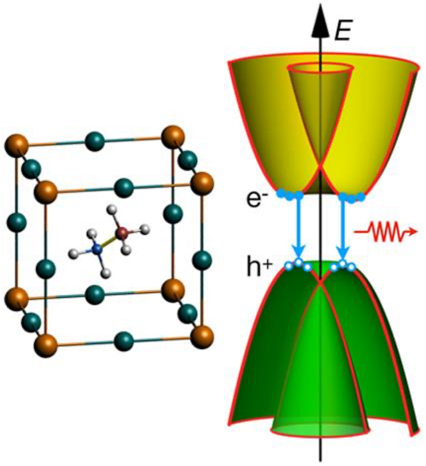
Researchers from the University of California, Santa Barbara used NERSC supercomputers to better understand the solar conversion efficiencies of hybrid perovskites and produce critical insights into how they work.

Significance and Impact

Hybrid perovskites are spectacularly efficient materials for photovoltaics. Just a few years after the first perovskite solar cells were fabricated, they have already achieved solar conversion efficiencies greater than 22 percent. Interestingly, the fundamental mechanisms that are responsible for this high efficiency are still being vigorously debated. The results of this study showed that a frequently cited explanation, based on low radiative rates, was not viable. This now provides a sound basis for future accurate modeling and design.

Research Details

Using more than 1,000 nodes on NERSC's Cori supercomputer, the team not only disproved one explanation for high solar cell efficiencies, but also studied how the materials could be used in light emitting diodes (LEDs). "These calculations are extremely demanding, and the compute power provided by NERSC has been instrumental in obtaining these results," commented lead researcher Chris Van de Walle.



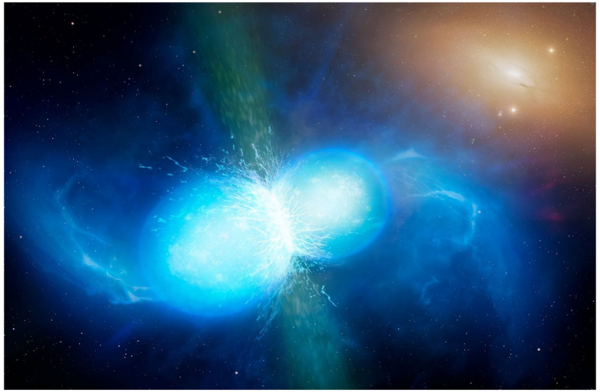
Strong spin-orbit coupling in halide perovskites induces splitting of the band edges, which could affect recombination rates.
Image credit: X. Zhang and J.-X. Shen.

*X. Zhang, J.-X. Shen, W. Wang, and C. G. Van de Walle, "First-Principles Analysis of Radiative Recombination in Lead-Halide Perovskites"; ACS Energy Letters **3**, 2329 (2018). 10.1021/acsenergylett.8b01297*

New Constraints on the Size of Neutron Stars

Scientific Achievement

Using a combination of state-of-the-art calculations of matter at extreme densities with gravitational-wave and electromagnetic observations of neutron stars and binary neutron star mergers, scientists have determined – with unprecedented accuracy – that a neutron star with 1.4 times the mass of our Sun is packed into a sphere 11.75 km in radius. The researchers also derived a value of 66.2 km/s/Mpc for the Hubble Constant, H_0, which characterizes the expansion rate of the Universe. The results were reported in 2020 in the journals Nature Astronomy and Science. The theoretical nuclear-physics research that contributed to this finding was led by Ingo Tews from Los Alamos National Laboratory and relied on NERSC's Cori supercomputer to generate the results.



An artist's impression of the collision of two neutron stars. This collision causes gravitational waves, a gamma-ray burst, and a massive explosion. Image courtesy of ESO/University of Warwick/Mark Garlick

Significance and Impact

Neutron-star mergers teach us about the nature of the densest matter in the Universe and can now be observed in both gravitational waves and various frequencies of light. These "multimessenger" observations together with accurate nuclear-physics calculations allowed scientists to better understand neutron stars and their properties, reducing the uncertainty of the radius of a 1.4 solar mass neutron star, which had previously been determined to be 10-14 km. The study also provided an independent measurement of H_0, the precise value of which is a subject of intense research. The value quoted in the Science paper is closely aligned with that derived from measurements of the Cosmic Microwave Background. The Nature paper also found that while mergers between two neutron stars can produce visible light, mergers between a black hole and a neutron star most likely will not.

Research Details

Using Cori, the research team applied "chiral effective field theory" to accurately calculate how nuclear matter behaves under the extreme conditions encountered in a neutron star, a teaspoon of which would weigh about 1 billion tons on Earth. Combining quantum Monte Carlo calculations of the "equation of state" – which ultimately determines the neutron star radius – with various observational constraints, the team was able to derive a value for the radius with an accuracy of less than 10%. Tews and his team used the auxiliary field diffusion Monte Carlo method, which employs statistical means to calculate the properties of dense nuclear matter. This code has very good scaling properties, which makes it ideally suited for NERSC's Cori supercomputer.

Capano, Collin D.; Tews, Ingo; et al., "Stringent constraints on neutron-star radii from multimessenger observations and nuclear theory"; NATURE ASTRONOMY, 4:625-632; 2020 JUN, 10.1038/s41550-020-1014-6

Dietrich, Tim; et al., "Multimessenger constraints on the neutron-star equation of state and the Hubble constant"; SCIENCE, 370:1450-1453; 2020 DEC 18, 10.1126/science.abb4317

Urban Landscapes Enhance Destructive Storms

Scientific Achievement

Using NERSC supercomputers to model destructive thunderstorms, researchers from Pacific Northwest National Laboratory found that urban landscapes and human-made aerosols – particles suspended in the atmosphere – can make wind gusts stronger, rain heavier, and hail larger and even steer storms toward cities.

Significance and Impact

Urbanization has been a significant change in the earth's environment since industrialization and is expected to further expand during the coming decades. Many modeling and observational studies have shown that landscapes can impact weather and climate, and it is important to understand how this will affect the lives of millions of Americans.

Research Details

Researchers modeled two large historical storms: a supercell near Kansas City that produced hail, strong wind, and a tornado; and a sea-breeze-induced thunderstorm near Houston. Using a version of the Weather Research and Forecasting model that includes routines to model aerosols and detailed chemistry and physics, the team found that storms were stronger when urban landscapes and human-produced aerosols – for example, from auto exhausts or farming – were included in the simulations. In addition to harnessing the computational power of NERSC's Cori supercomputer, the team also relied on a special allocation of 50TB of data storage on Cori's high-speed file system.

Fan, J.; Zhang, Y.; Li, Z.; Hu, J.; Rosenfeld, D., "Urbanization-induced land and aerosol impacts on sea-breeze circulation and convective precipitation"; Atmospheric Chemistry and Physics, 20:14163-14182; 2020 , 10.5194/acp-20-14163-2020

Fast-Charging, Safer Batteries

Scientific Achievement

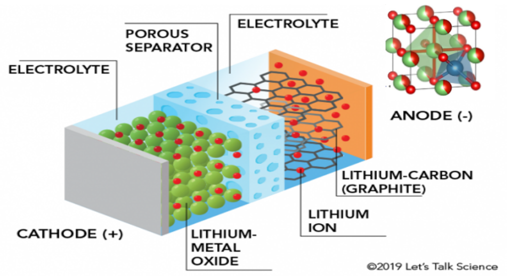
With the help of NERSC supercomputers, scientists from UC San Diego have developed a new material that makes batteries safer, holds more charge and charges faster compared to batteries commonly in use today. The study, which combined experimental and computational results from multiple user facilities, was published in the journal *Nature*.

Significance and Impact

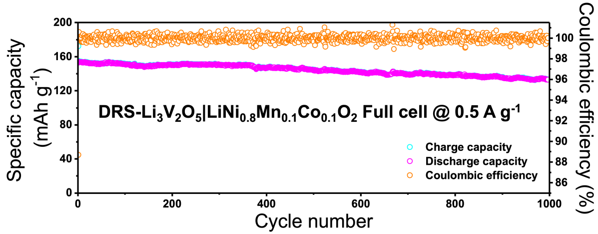
Rechargeable Lithium-ion batteries are pervasive in our lives today and scientists are working to make them more capable, safer, and convenient for a wide variety of applications from cell phones to laptops to electric vehicles. One of the common materials used in the negative terminal of a battery, the anode, is graphite, which can be subject to fire and explosions. An alternative, lithium titanate, is safer and faster to charge, but needs to be recharged often. In this study a disordered rock salt composed of Lithium, Vanadium, and Oxygen is described that charges quickly, is safer than graphite and holds more energy than Lithium titanate. It can also be charged and recharged more than 1,000 times with negligible capacity loss. The researchers have formed a company to commercialize the discovery.

Research Details

NERSC resources were used extensively in this work to perform Density Functional Theory (DFT) calculations that elucidated the unique mechanism for Li insertion into the material, as well as for the low migration barriers responsible for its fast charging capabilities. The study also used data computed by the Materials Project, which uses Cori as well.



Structure of a Lithium Ion Battery



This figure shows the extraordinary cycling stability of DRS-Li3V2O5 anode. Source: S.P Ong & Z. Zhu

Liu, H.; Zhu, Z.; Yan, Q.; Yu, S.; He, X.; Chen, Y.; Zhang, R.; Ma, L.; Liu, T.; Li, M.; Lin, R.; Chen, Y.; Li, Y.; Xing, X.; Choi, Y.; Gao, L.; Cho, H.S.-Y.; An, K.; Feng, J.; Kostecki, R.; Amine, K.; Wu, T.; Lu, J.; Xin, H.L.; Ong, S.P.; Liu, P., "A disordered rock salt anode for fast-charging lithium-ion batteries"; Nature, 585:63-67; 2020 , 10.1038/s41586-020-2637-6

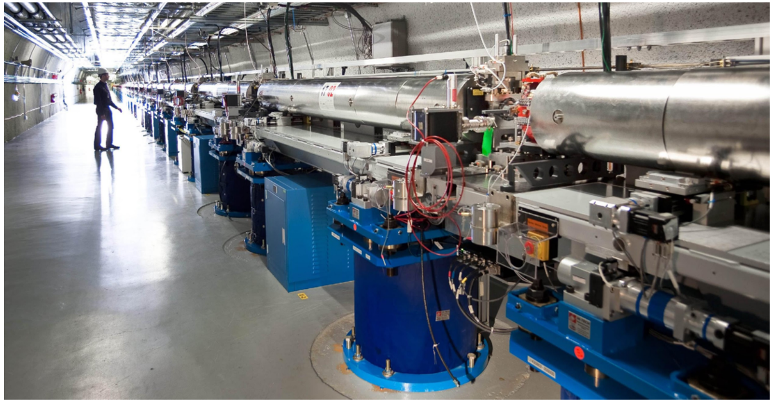
NERSC & LCLS Team Up on SARS-CoV-2 Research

Scientific Achievement

NERSC and researchers at the SLAC National Accelerator Laboratory connected in real time to allow researchers at the newly upgraded LCLS to conduct analysis that informed decision making while experimental runs were in progress. The collaboration allowed scientists to study the SARS-CoV-2 virus that causes COVID-19 in unprecedented detail.

Significance and Impact

The COVID-19 pandemic has sickened and killed many worldwide and caused widespread disruption in lifestyle and the world economy. A detailed understanding of the SARS-CoV-2 virus' structure and lifecycle is critical to developing vaccines and therapeutics.



Researchers working at the Linac Coherent Light Source used X-ray crystallography to capture detailed images of the structure of the SARS-CoV-2 virus.

Research Details

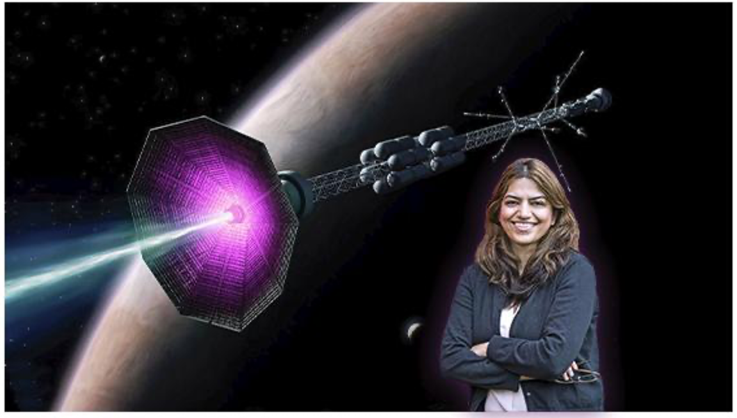
- A team led by Hasan DeMirci's group at Koç University used LCLS to study two crystal forms of the SARS-CoV-2 main protease at near-physiological temperature, which offers invaluable information for drug-repurposing studies.
- LCLS/SLAC, NERSC, and LBNL's Computational Research Division built an optimized pipeline that included improved communication, I/O, seamless portability from LCLS to NERSC using containers, customized job submission for optimized node sharing, and memory allocation.
- During a second run, researchers studied the atomic structure, dynamics, and function of the main protease and a papain-like protease at room temperature, which scientists hope could lead to development of an anti-viral treatment.
- The collaboration used LCLS to determine the time-resolved atomic structure from a slurry of microcrystals to which the drugs are added.
- The ability to process data in near to real time with access to resources at NERSC was essential for the team's decision making processes during the beamtime.

NERSC Project PI: Amedo Perazzo, SLAC
DOE Mission Science, Research Funded by Office of Basic Energy Sciences

Rocket Thruster Could Propel Humans to Mars and Beyond

Scientific Achievement

A scientist at Princeton Plasma Physics Laboratory (PPPL) has proposed a new type of rocket thruster that could take humankind to Mars and beyond, based on calculations performed on NERSC's Cori supercomputer. Fatima Ebrahimi, a research physicist at PPPL, showed that the proposed plasma thruster can generate exhaust with velocities of hundreds of kilometers per second (km/s). The device would apply magnetic fields to cause particles of plasma to shoot out the back of a rocket and, because of the conservation of momentum, propel the craft forward.



Princeton physicist Fatima Ebrahimi withan artist's conception of a rocket powered by plasma exhaust. The energetic plasma is created through magnetic reconnection, a process that occurs in the Sun and in fusion reactors.

Significance and Impact

Current space-proven plasma thrusters use electric fields to propel the particles, but they can only produce low specific impulse, which limits their speed. The recent Mars Perseverance Rover was traveling at about 5 km/s when it reached Mars, for example. If successfully implemented the proposed thruster could reduce travel time to Jupiter from 6 years to a matter of months.

Research Details

- A set of complex, high-resolution simulations of plasma physics were needed to confirm the efficiency of the magnetic reconnection design.
- Over the course of several weeks, Ebrahimi was able to run multiple simulations that could reproduce the higher forces generated by the engine.
- These high-resolution scans were able to prove that the engine would, in fact, generate higher levels of propulsion.

Ebrahimi, Fatima, "An Alfvenic reconnecting plasmoid thruster"; JOURNAL OF PLASMA PHYSICS, 86 2020 DEC 21, 10.1017/S0022377820001476

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC Project PI: Amitava Bhattacharjee, Princeton University
DOE Mission Science, Research Funded by Office of Fusion Energy Sciences

BERKELEY LAB

Regional Simulations of Building Response to Major Earthquakes

Scientific Achievement

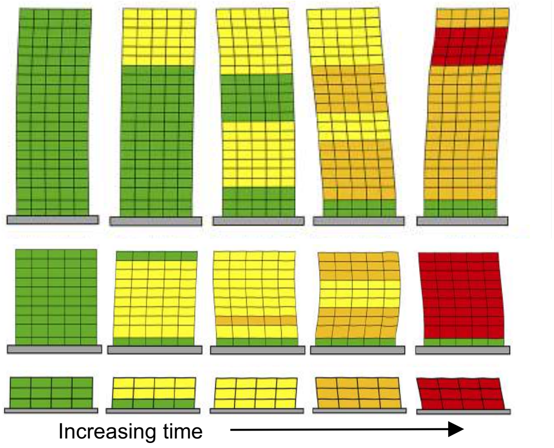
Using the EQSIM fault-to-structure computational framework running on NERSC's Cori supercomputer, a research team from the University of Nevada-Reno, Berkeley Lab, UC Berkeley, and Livermore Lab are providing new insights into how buildings respond to major earthquakes over large regions.

Significance and Impact

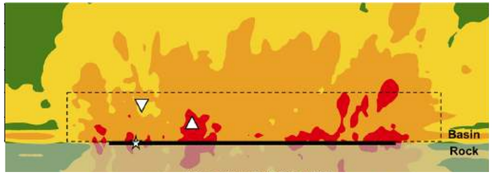
The risk to buildings and other structures over a geographical area due to major earthquakes is poorly understood. The effect on buildings depends on many complex factors, including where and how a fault ruptures, how the waves move through the Earth, and how the soil underneath the building interacts with the structure. This teams' simulation framework, leveraging the computational capability of Cori, allows researchers to examine many scenarios of interest and inform civic planners so they can save lives and protect infrastructure.

Research Details

- The team, lead by David McCallen from UNR and Berkeley Lab, simulated a magnitude 7.0 earthquake and looked in detail at the response of buildings of various sizes throughout a region.
- Using an allocation of computer time from the NERSC Director's Discretionary Reserve, the team ran the EQSIM framework, which is being developed with funding from the DOE Exascale Computing Project, on Cori using 2,048 nodes (139,000 processor cores). The project used 65 million hours of compute time in 2020.



New simulations provide insight into how earthquakes stress and distort buildings depending on their location, size, and shape. Red indicates the most distortion and green the least. Steel frame buildings were considered in this study.



Maps reveal the complex spatial distribution of distortions suffered by buildings following an earthquake.

McCallen, D.; Petrone, F.; Miah, M.; Pitarka, A.; Rodgers, A.; Abrahamson, N., "EQSIM—A multidisciplinary framework for fault-to-structure earthquake simulations on exascale computers, part II: Regional simulations of building response"; Earthquake Spectra 2020 , 10.1177/8755293020970980

NERSC

National Energy Research Scientific Computing Center