Science Highlights

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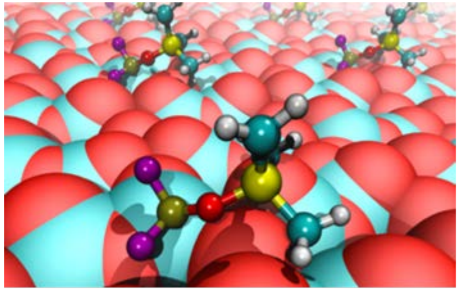

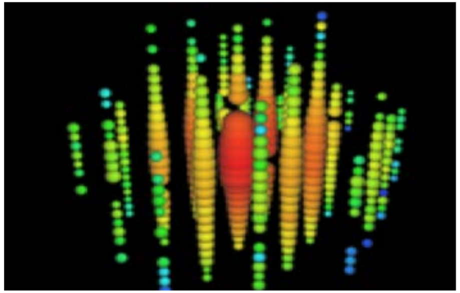

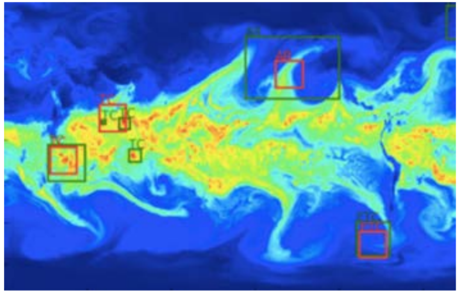

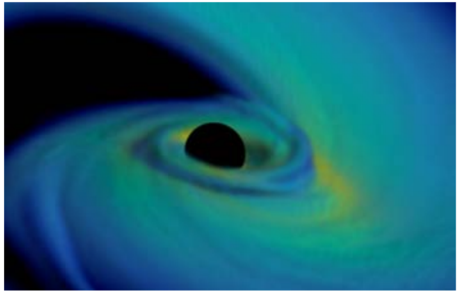

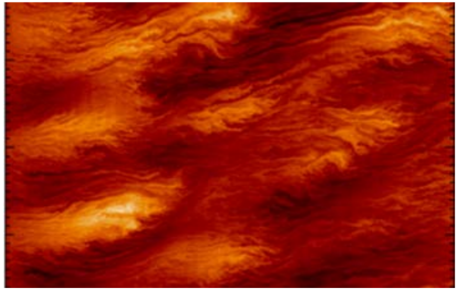

NERSC

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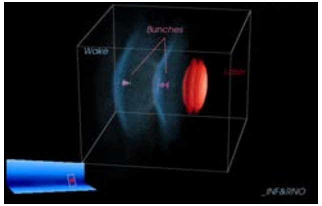
Science Highlights

Accelerator Physics

World record laser-driven plasma-based electron accelerator

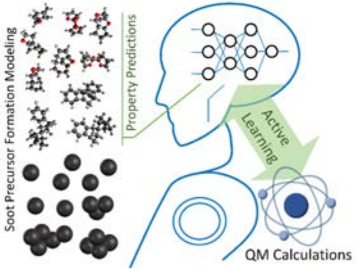
NERSC PI: J.-L. Vay, C. Benedetti , Berkeley Lab, *Physical Review Letters*

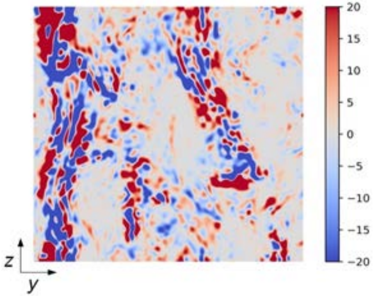


Chemistry

Enabling Thermochemistry Estimation using Deep Learning

NERSC PI: : William H. Green, MIT, *Journal of Physical Chemistry*

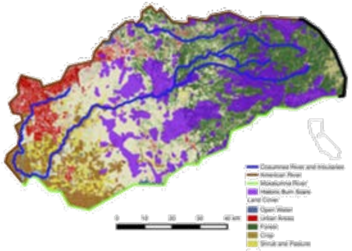




Physics

New Conservation Laws in Turbulent Magnetized Flows

NERSC PIs: Hussein Aluie, University of Rochester, *Physical Review Letters*



Environment

How California Wildfires Can Impact Water Availability

NERSC PI: Erica Siirila-Woodburn, Berkeley Lab, *Hydrological Processes*

Biochemistry

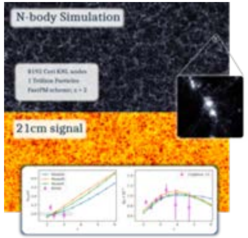
Turning On and Off a Heart Drug's Molecular Switch

NERSC PI: Yinlong Miao, U. of Kansas, *Proc. Nat. Acad. Of Sci.*

Cosmology

Mapping the Neutral Hydrogen in the Early Universe

NERSC PI: Yu Feng, UC Berkeley, *Journal of Cosmology and Astroparticle Physics*



World Record Laser-Driven Plasma-Based Electron Accelerator

Scientific Achievement

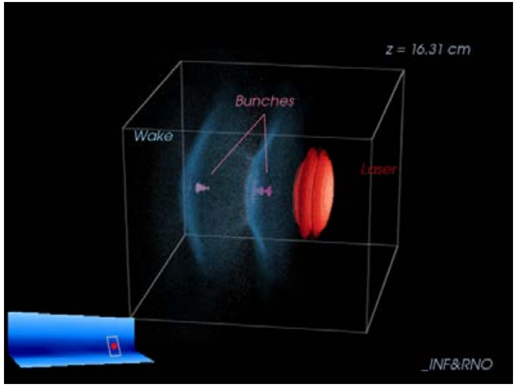
Guided by simulations performed at NERSC, researchers at Berkeley Lab's BELLA Center have set a new world record in laser-driven plasma-based electron acceleration by obtaining beams with an energy up to 7.8 GeV in a 20 cm-long plasma, nearly doubling their previous record. This result was made possible by the use of a new plasma target preparation technique where a "heater" laser pulse is used in combination with a discharge capillary to produce a deep enough plasma channel that is able to guide the laser.

Significance and Impact

Laser-plasma accelerators are able to accelerate particles to high energies over short distances, several orders of magnitude smaller than in conventional radio frequency technology. This could allow for compact, low-cost, accelerators for a variety of applications, including medical devices, security scanners, and probing the fundamental interactions of particle physics.

Research Details

The plasma channel produced by a capillary discharge was modified by a "heater" laser pulse used to reduce the on-axis density and increase the guiding strength of the channel. This allowed for the production of beams with an energy of up to 7.8 GeV in a 20 cm plasma. More than 15 million hours of computer time at NERSC were used to simulate the channel formation using the magneto-hydrodynamic code MARPLE and to model electron acceleration using the particle-in-cell code INF&RNO. These simulations were instrumental in understanding and optimizing the experiment.



Plasma waves (blue) excited by the PW BELLA laser pulse (red) as it propagates in a plasma channel. Background electrons are trapped and accelerated to an energy of up to 7.8 GeV in the plasma wave (pink/purple). Simulation performed with the Particle-In-Cell code INF&RNO (BLAST toolkit) at NERSC.

Gonsalves et al.,
Phys. Rev. Lett. 122, 084801 (2019),
doi.org/10.1103/PhysRevLett.122.084801

Enabling Thermochemistry Estimation using Deep Learning

Scientific Achievement

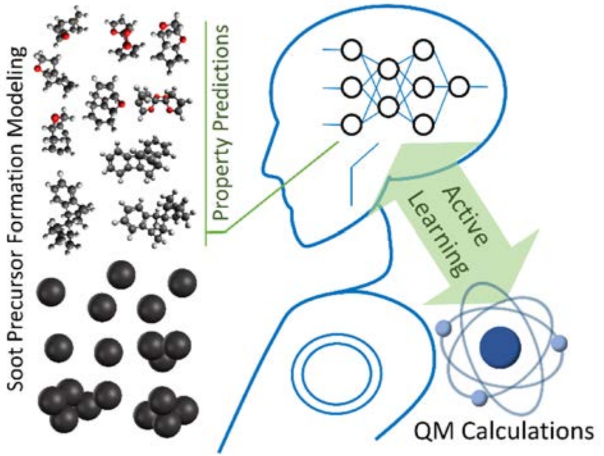
MIT researchers developed an automated system using an active learning process to continually perform quantum chemistry calculations using NERSC resources and retrain a deep learning model for predicting thermochemistry of complex polycyclic molecules.

Significance and Impact

Rapid estimation of thermochemistry is crucial in automated modeling of combustion and soot formation processes. In these cases, quantum chemistry is too expensive and conventional estimation methods do not easily adapt to unusual molecules. Using machine learning as a versatile estimator enables investigating more energy-efficient and environmentally beneficial processes.

Research Details

The research used the Cori supercomputer to spawn many quantum chemistry calculations ranging from density functional theory to high-level coupled cluster methods. Using a newly developed method for estimating uncertainty integrated into the machine learning model enabled automatic identification of new molecules for quantum chemistry calculations via an active learning scheme. Ongoing work involves improving the accuracy of the deep learning model by performing thousands of explicitly-correlated coupled cluster calculations and combining them with the existing model using transfer learning.



A self-evolving model that can adapt to a broad range of polycyclic soot precursors by integrating an active learning machine with automatic ab initio calculations.

NERSC staff built an OpenMP version of Q-Chem software to alleviate system issues caused by using an MPI-only version.

Li et al., Journal of Physical Chemistry A 2019,
doi: 10.1021/acs.jpca.8b10789

NERSC Project PI: William H. Green, MIT
DOE Mission Science, Funded by Offices of Basic Energy Sciences; Energy Efficiency & Renewable Energy, DARPA, & DOD

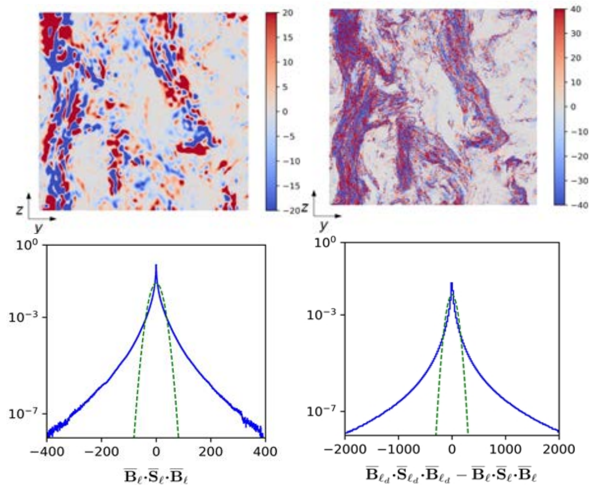
New Conservation Laws in Turbulent Magnetized Flows

Scientific Achievement

University of Rochester researchers used a novel coarse-graining framework for disentangling multiscale interactions to uncover two separate conservation laws over an entire range of length scales in turbulent magnetized flows. The work relied on a suite of massively parallel simulations run on NERSC.

Significance and Impact

Flows which are coupled to magnetic fields (MHD) are central to our understanding of a wide variety of systems ranging from the cosmological to the terrestrial. These include galaxies, nebulae, star formation, space weather, nuclear fusion, and metallurgy. The findings give us two dynamical invariants (kinetic energy and magnetic energy) instead of just one (total energy). Invariants are highly prized quantities from which the governing laws of motion are derived. The results have implications on the energetics and dissipation of these flows, magnetic reconnection such as in solar flares, magnetic amplification by dynamo action, and on modeling efforts such as in active galactic nuclei.



Massively parallel simulations were used to unravel the energy pathways in turbulent magnetized flows and find new conservation laws. Image: Xin Bian and Hussein Aluie, UofR

Research Details

The work relied on simulations using up to 8.5 billion grid-points on 16,384 computing cores over a month's worth of computing. It required ~6.3 million CPU-hours and generated > 6 Terabytes of data.

Bian, Xin; Aluie, Hussein, "Decoupled Cascades of Kinetic and Magnetic Energy in Magnetohydrodynamic Turbulence"; Physical Review Letters, 122 2019 APR 5, 10.1103/PhysRevLett.122.135101

How California Wildfires Can Impact Water Availability

Scientific Achievement

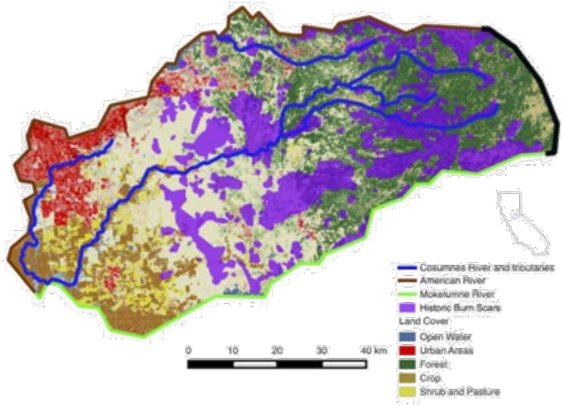
Berkeley Lab researchers used NERSC supercomputers to show that conditions left behind by California wildfires lead to greater winter snowpack, greater summer water runoff and increased groundwater storage.

Significance and Impact

In recent years, wildfires in the western United States have occurred with increasing frequency and scale. Even though California could be entering a period of prolonged droughts with potential for more wildfires, there is little known on how wildfires will impact water resources. The study is important for planners and those who manage California's water.

Research Details

The researchers modeled the Cosumnes River watershed, which extends from the Sierra Nevadas down to the Central Valley as a prototype of many California watersheds. Using about 3 million hours on NERSC's Cori supercomputer to simulate watershed dynamics over a period of one year the study allowed them to identify the regions that were most sensitive to wildfire conditions, as well as the hydrologic processes that are most affected.



Berkeley Lab researchers built a numerical model of the Cosumnes River watershed, extending from the Sierra Nevada mountains to the Central Valley, to study post-wildfire changes to the hydrologic cycle. (Credit: Berkeley Lab).

Maina, FZ, Siirila-Woodburn, ER. Watersheds dynamics following wildfires: Nonlinear feedbacks and implications on hydrologic responses. Hydrological Processes. 2019; 1– 18. https://doi.org/10.1002/hyp.13568

Turning On and Off a Heart Drug's Molecular Switch

Scientific Achievement

A research team from the University of Kansas and the University of California, San Diego, has shown for the first time details about how a key molecular switch, implicated in a variety of medical conditions including heart disease, is turned on and off.

Significance and Impact

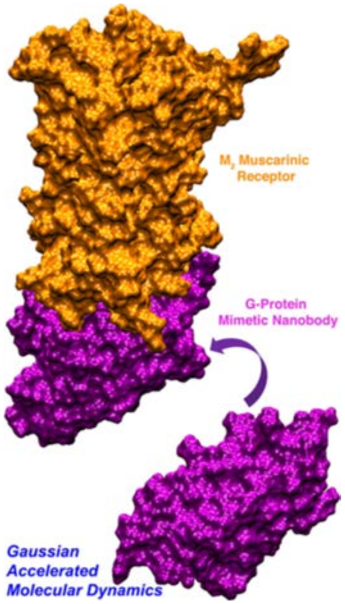
G-protein-coupled receptors (GPCR) are the largest and most diverse group of membrane receptors in animals, plants, fungi, and protozoa. Between one-third to one-half of all marketed drugs act by binding to GPCRs, treating diseases including cancer, asthma, schizophrenia, Alzheimer's and Parkinson's disease, and heart disease. This is the first molecular dynamics simulation for any GPCR-protein binding and provides important insights into the mechanism of GPCR–nanobody binding.

Research Details

The researchers used about 3 million hours on NERSC's Edison and Cori supercomputers to study binding to the "M_2" GPCR receptor. The simulations revealed pathways and important low-energy intermediate states of the G-protein mimetic nanobody binding, results that are consistent with experimental data and provide important insights into the binding mechanism.

Robust Gaussian accelerated molecular dynamics (GaMD) has unprecedentedly captured spontaneous binding of a G-protein mimetic nanobody to the M2 muscarinic G-protein-coupled receptor (GPCR). Image: Yinglong Miao, University of Kansas; J. Andrew McCammon, UC San Diego

Some Information for this slide was taken from a UCSD release.



Yinglong Miao, J. Andrew McCammon
Proceedings of the National Academy of Sciences Mar 2018, 115 (12) 3036-3041; DOI: 10.1073/pnas.1800756115

Mapping Neutral Hydrogen in the Early Universe

Scientific Achievement

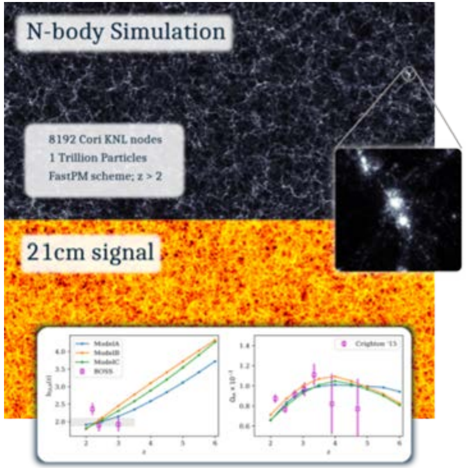
Researchers at the Berkeley Center for Cosmological Physics developed a model that produces maps of the 21 cm emission signal from neutral hydrogen in the early universe. Thanks to NERSC supercomputers, the team was able to run simulations with enough dynamic range and fidelity to theoretically explore this uncharted territory that contains 80% of the observable universe by volume and holds the potential to revolutionize cosmology.

Significance and Impact

One of the most tantalizing, and promising cosmic sources is the 21 cm line in the very early universe. This early time signal combines a large cosmological volume for precise statistical inference, with simple physics processes that can be more reliably modeled after the cosmic initial conditions. The model developed in this work is compatible with current observational constraints, and serves as a guideline for designing intensity mapping surveys and for developing and testing new theoretical ideas.

Research Details

The team developed a quasi-N-body scheme that produces high-fidelity realizations of dark matter distribution of the early universe, and then developed models that connects the dark matter distribution to the 21cm emission signal from neutral hydrogen. The simulation software FastPM was improved to run the HiddenValley simulation suite, which employs 1 trillion particles each, and runs on 8,192 Cori KNL nodes – **the largest N-body simulation ever carried out at NERSC**.



Upper panel: dark matter with an inset of the most massive galaxy system in the field of view. Lower panel: 21cm emission signal with an inset of the clustering properties compared with current constraints. Horizontal span: 1.4 comoving Gpc (6 billion light years); Thickness: 40 million light years.

Modi, Chirag; Castorina, Emanuele; Feng, Yu; White, Martin, "; Journal of Cosmology and Astroparticle Physics 2019 Sep, 10.1088/1475-7516/2019/09/024

National Energy Research Scientific Computing Center