Science Highlights

Released: Oct. 15, 2019

Science Highlights
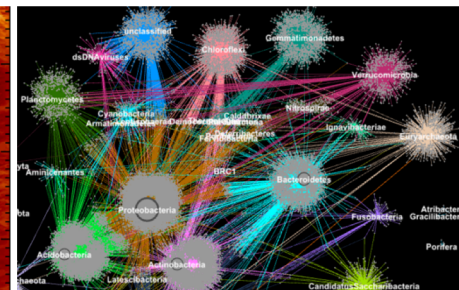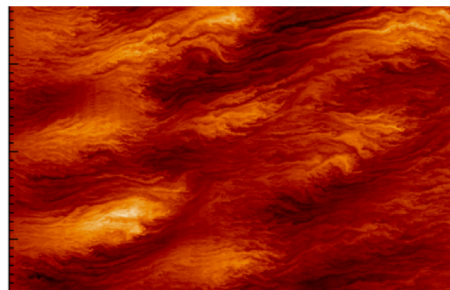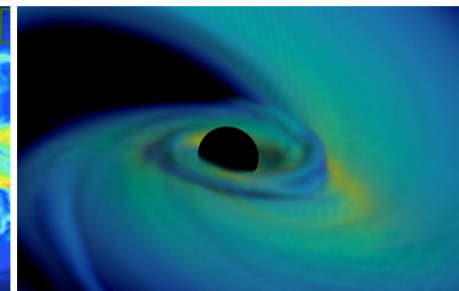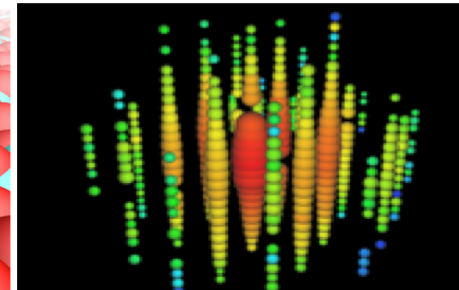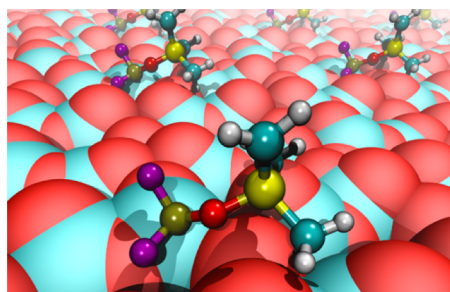
Fusion Energy

Towards Simpler Fusion Power Devices

NERSC PI: Chris Hansen, U. Washington, *Physics of Plasmas*
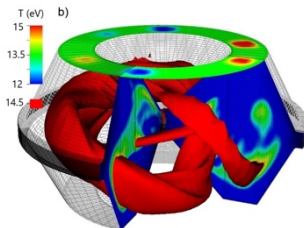
Materials

Exploring the Real-World Materials Genome

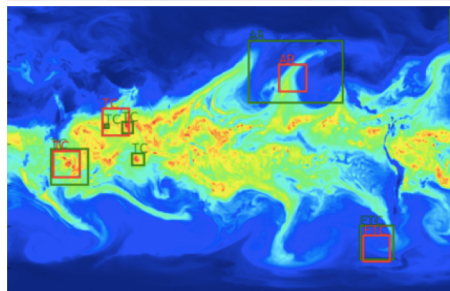**NERSC PI: C. Wolverton, Northwestern University,** *Phys. Rev. X*
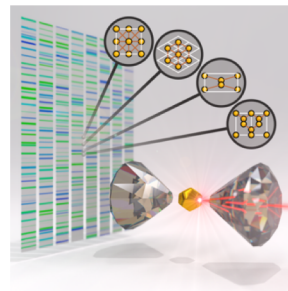
Earth Sciences

DOE Models Simulate Antarctic Ice Sheet Evolution

NERSC PIs: S. Price, LANL; E. Ng, Berkeley Lab; *Geosc. Model Dev. & Geophys. Res. Lett.*
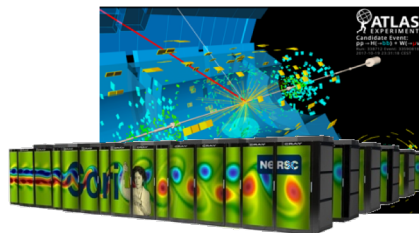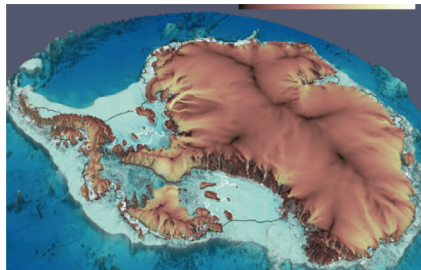
High Energy Physics

ATLAS Experiment: Scaling High Throughput Workflows

NERSC PI: J. Taylor Childers (ANL). *J. Phys.: Conference Series*

Materials

Machine-Learned Impurity Prediction in Semiconductors

NERSC PI: Maria K.Y. Chan, ANL, *Chem. Mat., ACS Appl. Mater. Interfaces*
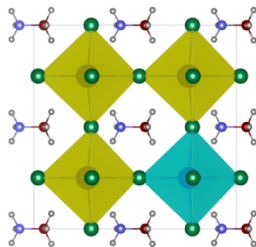
Astrophysics

Uncovering the Origins of Peculiar Supernovae

**NERSC PI: Wynn Jacobson-Galán, UCSC,** *Monthly Notices of the Royal Astronomical Society*

Released Oct. 25, 2019

Towards Simpler Fusion Power Devices

Scientific Achievement

Researchers at the University of Washington have modeled a magnetic confinement system with large-scale perturbations to further understand the role that these perturbations play in the self-organization of plasmas in fusion energy devices.

Significance and Impact

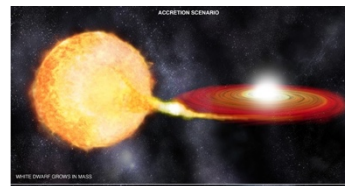Fusion power technology has the potential to produce electricity with minimal environmental effects, however the complexity of devices and associated cost are two major obstacles. Self-organized plasma equilibria devices like HIT-SI at the University of Washington could address both those challenges compared to conventional tokamak fusion devices, but first an increased understanding of the dynamics involved with large perturbations on a plasma equilibrium are required.

Research Details

A variety of simulations were performed, involving about 2 million NERSC hours, that have increased confidence in the predictive modeling of plasma self-organization processes with extended Magneto-Hydrodynamic codes. The work focused on obtaining agreement with experimental results observed when both the temporal (oscillation frequency) and spatial structure of the applied perturbations are changed.
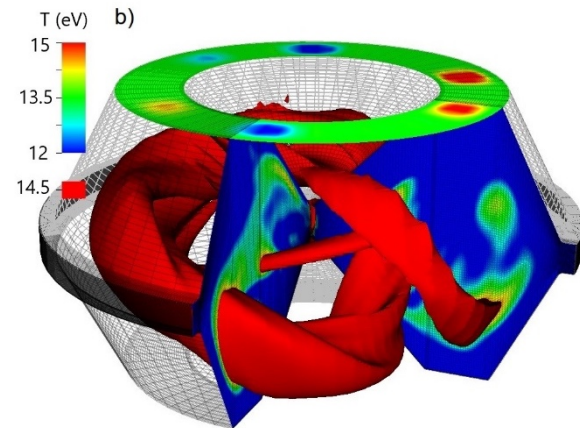
Simulations were performed to model large 3-D perturbations and the role they play on plasma self-organization on the HIT-SI device at the University of Washington.

NERSC consultants provided assistance to developers of the NIMROD code used in this work.

Scientific Achievement

Researchers at Northwestern University developed a novel computational framework that runs on NERSC's Cori supercomputer to rapidly explore apparent paradox of material phases that exist in nature that should be unstable according to calculations that assume idealized conditions of zero pressure and zero temperature. Using this method, the stability of these material phases is better understood, and the team has identified several new intermetallic high-pressure phases that can be realized with existing experimental techniques.

Significance and Impact

We are heading towards an age where materials are identified and designed with tailored properties to tackle global environmental challenges. Computational tools are key to this effort and the researchers' novel framework paves a route toward robust exploration of the entire materials genome.

Research Details

The researchers used their novel techniques in conjunction with calculated materials properties in the Open Quantum Materials Database (OQMD) to explain why some compounds remain relatively stable in the environment. Further, more than 3,500 new compounds that are stable at finite pressures were predicted. The investigation used 800,000 hours of compute time on Cori.
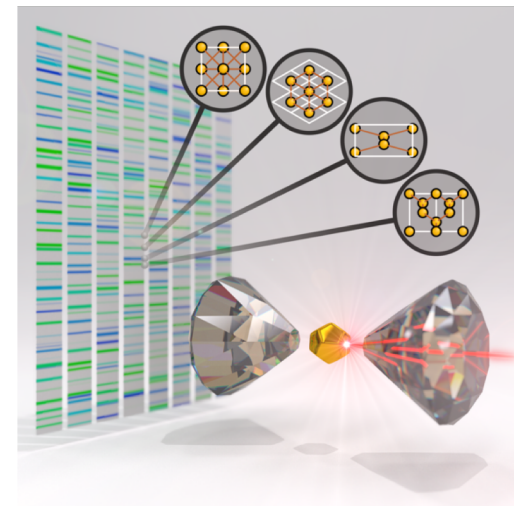
A new framework for predicting materials behavior at high pressure combines computational approximations with extant materials data to provide a tool for discovering new materials and their properties under nonambient pressure conditions.

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DOE Models Simulate Antarctic Ice Sheet Evolution


Scientific Achievement

Ice sheet models developed under a DOE SciDAC project and run at NERSC have contributed to three international model intercomparison projects focused on assessing the future evolution of the Antarctic ice sheet.

Significance and Impact

Results from one experiment, shown at right, provide an upper-bound estimate for the potential sea-level rise from Antarctica resulting from the rapid and sustained loss of all floating ice shelves. This process triggers the marine ice sheet instability, which is currently one of the largest sources of uncertainty in future sea-level projections.

Research Details

DOE's simulation results represent the highest resolution and highest fidelity simulations contributed to the project. Optimization methods are used to initialize DOE's MALI and BISICLES ice sheet models to match present-day observations. An extreme (and unrealistic) perturbation is then applied by instantaneously removing all of Antarctica's floating ice shelves. This triggers immediate, continuous, and unstable retreat of marine sectors of the ice sheet. The simulations used 10s of millions of hours on NERSC computers.
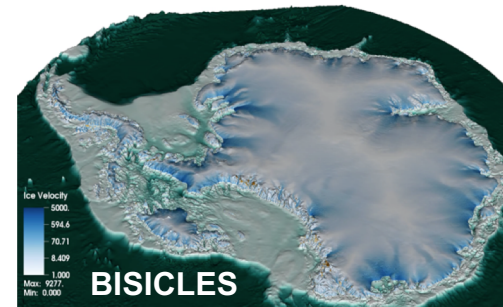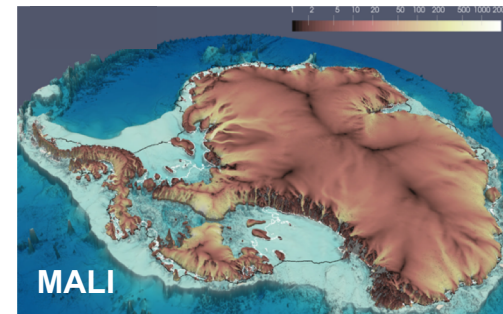
Simulated Antarctic ice sheet 200 years after all floating ice shelves are instantaneously removed.

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NERSC PI's: S. Price, Los Alamos National Lab; E. Ng, Lawrence Berkeley National Lab
DOE Mission Science, Funded by DOE Office of Biological & Environmental Research

Scientific Achievement

Researchers from the ATLAS experiment at the Large Hadron Collider (LHC) used NERSC's Cori supercomputer to simulate over 250 million proton collisions in support of the experiment's data analysis efforts. This campaign also paves the way for even larger analysis that will be needed following a 2025 LHC upgrade.

Significance and Impact

The LHC is the world's central laboratory for High Energy Physics research, where the ATLAS experiment observes the highest energy proton-proton collisions. Having discovered the Higgs Boson, the collaboration is now studying the Higgs with great precision with the goal of finding clues that lead to the next discovery. This project specifically targets running ATLAS simulation on DOE's HPC resources to prepare for dealing with an increase of 10-100X more data following the LHC upgrade.

Research Details

This was the third in a line of DOE ASCR Leadership Computing Challenge awards in which the ATLAS experiment has continued to improve the efficiency of simulation workflows at DOE HPC facilities. During this award period, the Harvester edge service was largely developed, deployed, and validated for production. This was an important step for the experiment. Harvester runs on a login node and retrieves ATLAS simulation jobs from the PanDA workflow system and marshals the work through the local resource. The MPI-enabled workload, Yoda, was also under development to improve efficiency of ATLAS applications.
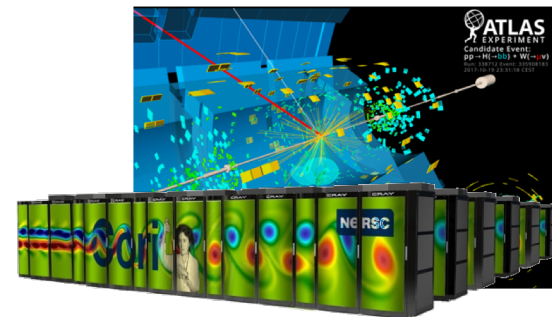
ATLAS Experiment made heavy use of NERSC in 2017-18 to analyze data and prepare for LHC upgrades.

NERSC worked to make itself act like a standard Worldwide LHC Computing Grid site. NERSC's shifter software with docker support enabled scaling ATLAS's large complicated software stack.

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NERSC Project PI: J. Taylor Childers, Argonne National Lab
DOE Mission Science, Research Funded by Office of High Energy Physics

BERKELEY LAB

Machine-Learned Impurity Prediction in Semiconductors

Scientific Achievement

Argonne National Laboratory researchers ran high-throughput simulations on NERSC supercomputers and generated comprehensive datasets of impurity properties in two classes of semiconductors: lead-based hybrid perovskites and cadmium-based chalcogenides. These datasets led to machine learned models that enable accelerated prediction and design for the entire chemical space of materials and impurities in these semiconductor classes.

Significance and Impact

Impurity energy levels in semiconductors can change their behavior in ways that have important consequences for solar cell applications. The ability to instantly and accurately estimate such impurity levels is paramount. The current research combines simulation and machine learning to generate results that can potentially transform the design of novel semiconductors that are defect-tolerant or have tailored impurity properties.

Research Details

The researchers performed density functional theory calculations for hundreds of impurity atoms in selected semiconductors to determine their formation enthalpies and energy levels. The results were transformed into predictive models using machine learning algorithms. The DFT simulations modeled systems containing ~ 100 atoms, using ~ 1.5 million CPU hours.
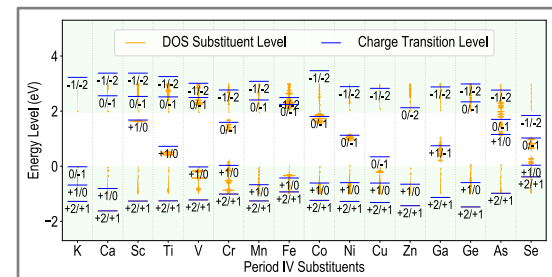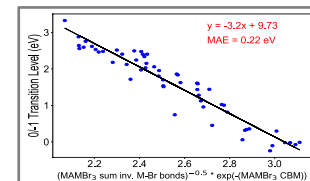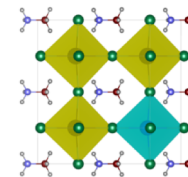
High-throughput DFT data was generated for impurity energy levels in semiconductors (example shown for a hybrid perovskite above), which lead to machine-learned predictive models.

A. Mannodi-Kanakkithodi et al., "Comprehensive Computational Study of Partial Lead Substitution in Methylammonium Lead Bromide", accepted, Chem. Mater. doi: 10.1021/acs.chemmater.8b04017 (2019).
D.H. Cao et al., "Charge Transfer Dynamics of Phase Segregated Halide Perovskite mixtures", ACS Appl. Mater. Interfaces, 11 (9), pp 9583–9593 (2019).

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BERKELEY LAB

# Uncovering the Origins of Peculiar Supernovae

Scientific Achievement

Astrophysicists at the University of California, Santa Cruz have constrained the type of binary star system responsible for a new, under-luminous stellar explosion called a Type Iax supernova. With supercomputers at NERSC, the research team was able to link observed helium in these objects to the proposed formation channel of a white dwarf star accreting mass from a helium star companion.

Significance and Impact

Thermonuclear supernova explosions (e.g., Type Iax) create most of the heavy elements within the universe and play a crucial role in the lives of binary star systems. Type Iax supernovae are a new class of stellar explosion whose progenitor star system is still relatively unknown. Determining the origins of these supernovae aids in our understanding of stellar evolution and the mechanisms responsible for these incredible explosions.

Research Details

Researchers modeled the dynamic properties of each ion present the supernova spectra. These unique fitting routines helped to describe the elements produced in the explosion, with an emphasis on identifying ionized helium. Detections of helium in spectral models were then used to explain how a White Dwarf + Helium Star progenitor system can produce these particular explosions. For 6 months, the team's NERSC simulations modeled the spectral data of over 100 Type Iax supernova observations, using ~300,000 CPU hours.
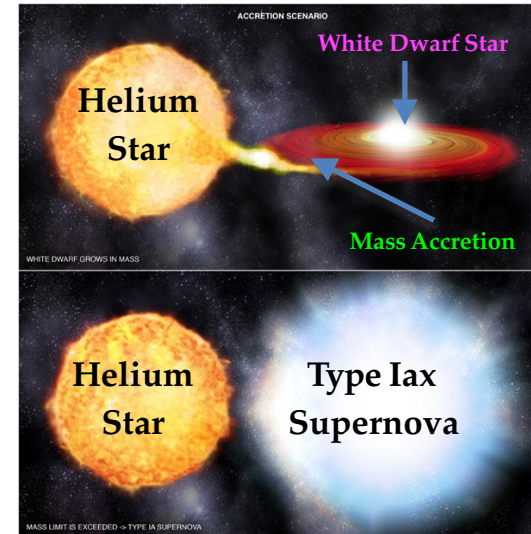
NERSC simulations modeled the elemental composition of all known Type Iax supernova explosions. The ions detected in these explosions helped confirm the explosion scenario shown above. Image: Wikipedia Commons and Discovery Magazine

National Energy Research Scientific Computing Center