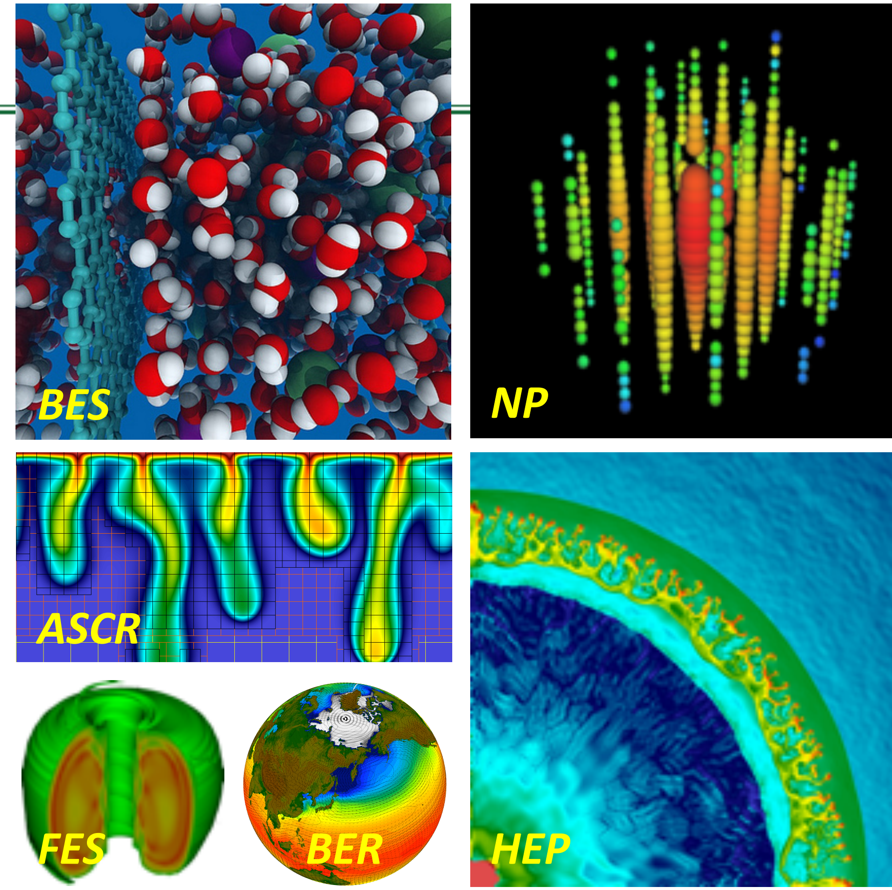
NERSC Science Highlights

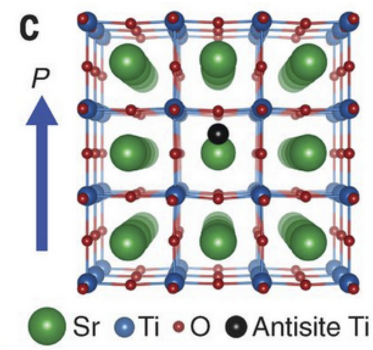


NERSC

December 2015

U.S. DEPARTMENT OF ENERGY | Office of Science

Science Highlights December 2015

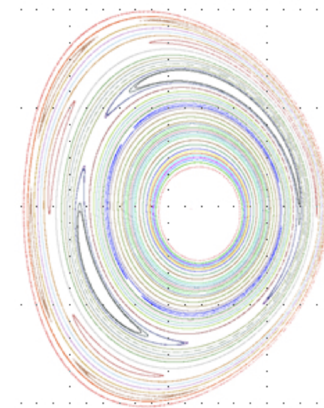


Materials Science

Theoretical calculations help provide evidence of room-temperature ferroelectricity in nanometer-thick films
(Xifan Wu , Temple Univ., *Science*)

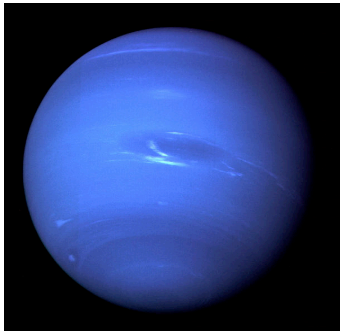
Fusion Energy

3D simulations run at NERSC help gain new insights into fusion plasma behavior that will improve the ability to stabilize a tokamak reactor
(S. Jardin , Princeton Plasma Physics Lab, *Phys. Rev. Lett.*)



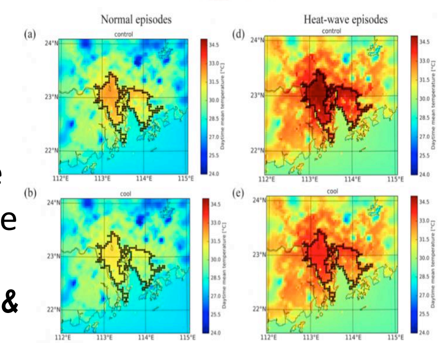
Chemistry

Simulations run at NERSC lead to the prediction of a new phase of superionic ice, a special form of ice that could exist on Uranus and Neptune
(**Roberto Car , Princeton U., *Nature Comm.)***



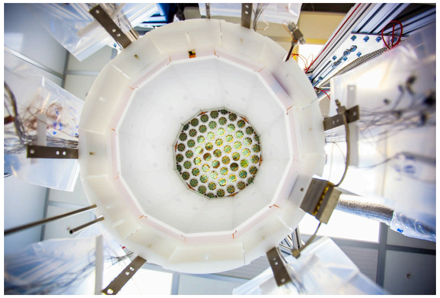
Energy

Computer models run at NERSC determine that, during a heat wave, white roofs can help mitigate the urban heat island effect
(Dev Millstein , LBNL, *Env. Sci. & Tech.)*



High Energy & Nuclear Physics

Simulations run at NERSC are helping the Large Underground Xenon (LUX) dark matter experiment better focus their search for dark matter particles
(R. Jacobsen , LBNL, Phy. Rev. Lett.)



Creating Nanoscale Ferroelectricity from a Nonferroelectric Film

Scientific Achievement

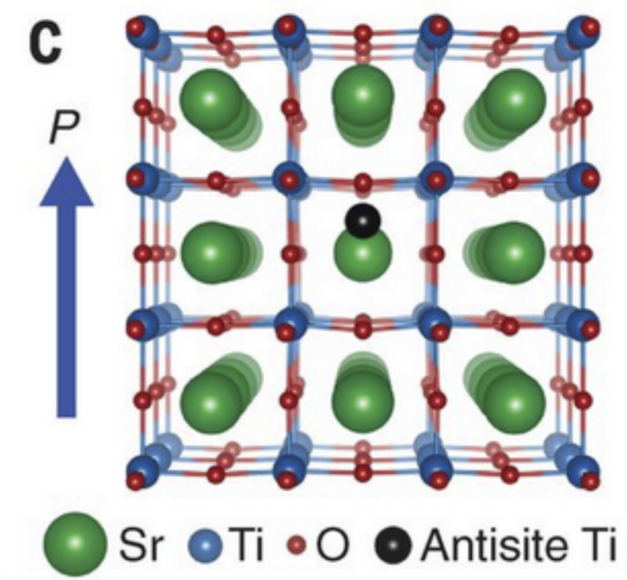
A combination of theoretical calculations, electrical measurements and structural analyses has provided evidence of room-temperature ferroelectricity in nanometer-thick films

Significance and Impact

Thin ferroelectric films are needed in computers and medical devices, but they typically become less polarized the thinner they become

Research Details

- The research team worked with a non-ferroelectric material – strontium titanate ($SrTiO_3$) – that has naturally occurring polar nanoregions (PNRs). As the film became thinner, they found that when the thickness reached the typical size of the PNR regions, the whole film aligned and became ferroelectric.
- Density functional theory models run on NERSC's Edison system were critical in helping the researchers understand the energy characteristics of $SrTiO_3$, while phase-field simulations were used to model polarization in a representative PNR region.



Theoretical calculations run at NERSC helped provide evidence of ferroelectricity in ultrathin films in otherwise nonferroelectric $SrTiO_3$.

D. Lee, H. Lu, Y. Gu, et al.
Science, September 2015, Vol. 349, Issue 6254, pp. 1314-1317

Stabilizing a Tokamak Plasma

Scientific Achievement

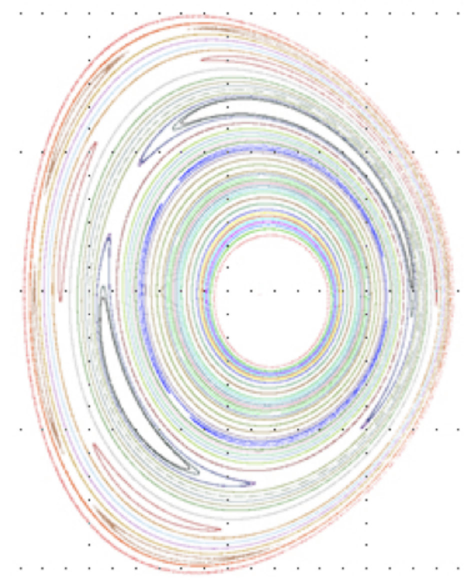
3D simulations run at NERSC helped an international team of physicists gain new insights into fusion plasma behavior that will improve the ability to stabilize plasma in a tokamak reactor

Significance and Impact

Learning how to model and study the behavior of fusion plasmas has important implications for the design and functionality of ITER, the multinational fusion facility being constructed in France

Research Details

- Physicists from Princeton Plasma Physics Laboratory, General Atomics and the Max Planck Institute for Plasma Physics used NERSC's Edison computer and M3D-C1, a program that creates 3D simulations of fusion plasmas to determine that, under certain conditions a helix-shaped whirlpool of plasma forms around the center of the tokamak.
- The swirling plasma acts like a dynamo—a moving fluid that creates electric and magnetic fields. Together these fields prevent the current flowing through plasma from peaking and crashing.



A cross-section of the virtual plasma showing where the magnetic field lines intersect the plane. The central section has field lines that rotate exactly once. Image: Stephen Jardin

S.C. Jardin, N. Ferraro, I. Krebs
Phys. Rev. Lett. 115, 215001, November 2015

Predicting a New Phase of Superionic Ice

Scientific Achievement

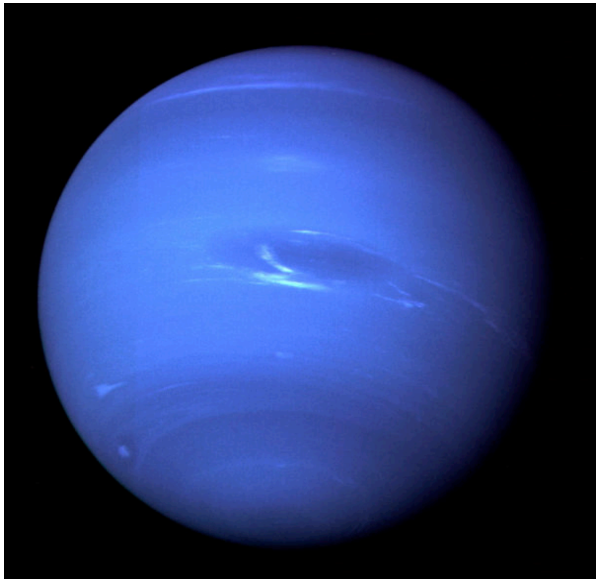
Simulations run at NERSC enabled researchers at Princeton University to model states of superionic ice that would be difficult to study experimentally

Significance and Impact

Their calculations led to the prediction of a new phase of superionic ice, a special form of ice that could exist on Uranus and Neptune

Research Details

- Unlike water or regular ice, in superionic ice the water molecules dissociate into charged atoms (ions), with the oxygen ions locked in a solid lattice while the hydrogen ions move like the molecules in a liquid.
- The researchers calculated the ionic conductivity of each phase of superionic ice and found unusual behavior at the transition where the low temperature crystal, in which both oxygen and hydrogen ions are locked together, transforms into superionic ice.



Unlike Earth, which has two magnetic poles, ice giants such as Neptune (pictured) can have many local magnetic poles, which could be due to superionic ice and ionic water in the mantle of these planets. Image: NASA

J. Sun, B.K. Clar, S. Torquato, R. Car
Nature Communications, 6, 8156, August 2015

LUX Dark Matter Experiment

Scientific Achievement

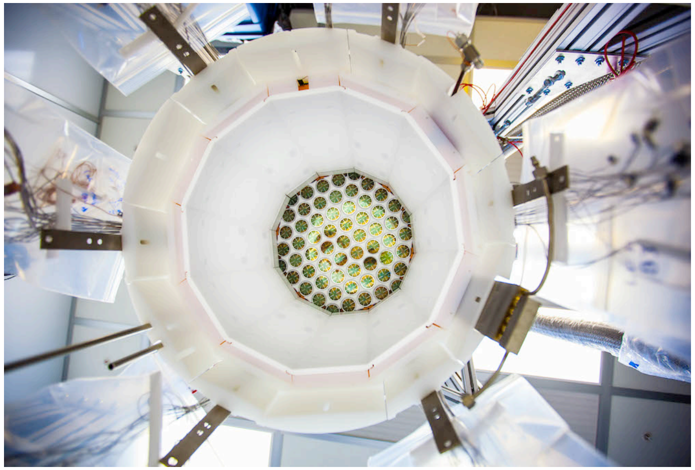
Simulations run at NERSC are helping the Large Underground Xenon (LUX) dark matter experiment better focus their search for dark matter particles

Significance and Impact

The findings help rule out the possibility of dark matter detections at low-mass ranges where other experiments had previously reported potential detections

Research Details

- LUX researchers are looking for WIMPs (weakly interacting massive particles), which are among the leading candidates for dark matter
- Improvements in LUX calibration, coupled with computer simulations run on NERSC's Edison supercomputer, allowed scientists to test additional particle models of dark matter that now can be excluded from the search
- NERSC also stores large volumes of LUX data—measured in trillions of bytes (terabytes)—on an ongoing basis.



A view inside the LUX detector.

LUX Collaboration,
Phys. Rev. Lett., Dec. 11, 2015

Reflective Roofs Help Reduce Energy Use

Scientific Achievement

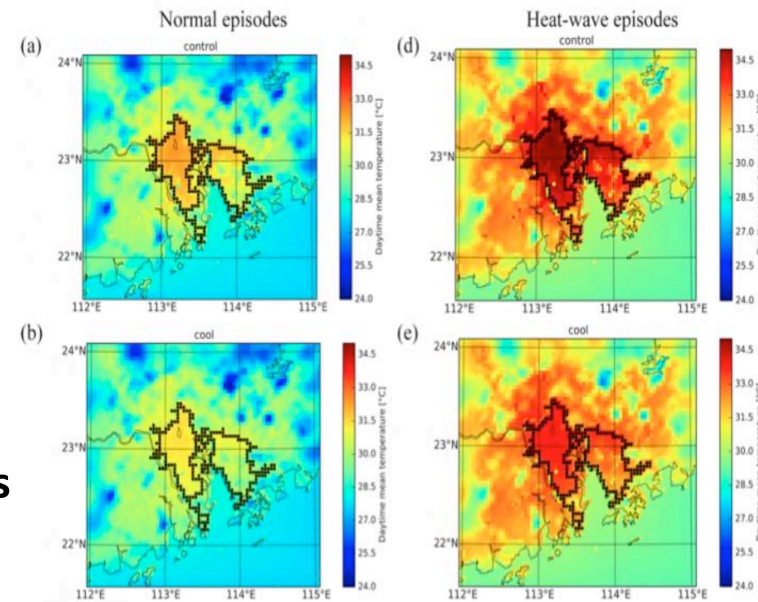
Berkeley Lab and Chinese researchers used computer models run at NERSC to determine that, during a heat wave, white roofs can help mitigate the urban heat island effect

Significance and Impact

Reflective roofs can substantially reduce energy use and greenhouse gas emissions in climate zones with hot summers

Research Details

- Guangzhou is a sprawling megacity in southern China with a population of more than 8.5 million. The researchers simulated conditions from six of the strongest historical heat waves over the last decade and compared them to 25 typical summer weeks between 2004 and 2008.
- Using a regional climate model and an urban model to adjust roof reflectance, they found that the average urban midday temperature was lowered by 1.2 degrees C (2.2 degrees F) during heat waves, or 50% more than the 0.8 degrees C reduction for typical summer conditions.



The greater urban area of Guangzhou is outlined in the center of each figure. A midday urban heat island effect is clearly visible. The results of increased roof albedos are shown in the bottom row.

D. Millstein, R. Levinson, P. Rosado, M. Cao, Z. Lin
Environmental Science & Technology,
November 2015, 49, 14672-14679

BER PI: Dev Millstein (LBNL)