NERSC Science Highlights

A selection of recent results

March 2012

Scientific Accomplishments at NERSC
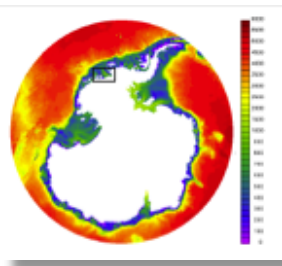
Climate
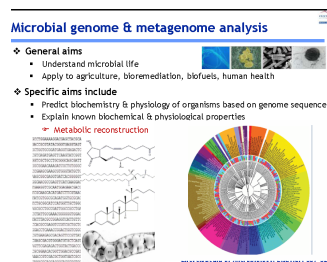
NERSC resources are being used to conduct pathbreaking simulations of decade-to-century-scale ice sheet evolution.
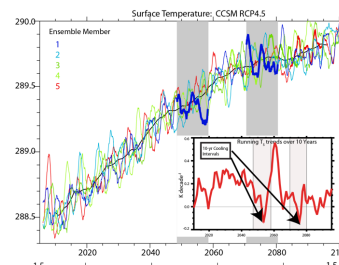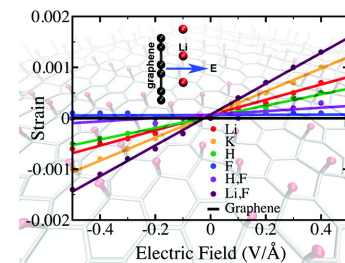**(W. Collins, LBNL)**

Materials

Calculations explain "designer" piezoelectric effects in graphene; could yield dramatic degree of control in nanotechnology
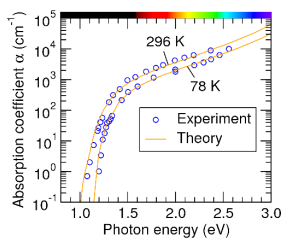**(E. Reed, Stanford)**

Genomes

Genomes pipeline at NERSC can process 100 million genes in few days, a task that used to require weeks at the JGI.
(V. Markowitz, LBNL)

Climate

Key finding that deep oceans can mask global warming for decade-long periods
(G. Meehl, A. Hu, NCAR)

Solar Energy

A NERSC "NISE" award and software by a NERSC consultant yield an important new method for characterizing solar energy materials.
(E. Kioupakis, U. Michigan)

High Energy Physics

An important piece of the neutrino puzzle has fallen into place, thanks to data transfer, storage, analysis, archive, and gateway capabilities at NERSC and ESnet.
**(K.-B. Luk, LBNL)**

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BERKELEY LAB — Lawrence Berkeley National Laboratory

# Science at Scale: Simulations Aid in Understanding Climate Impacts

- **Interaction between warming ocean and Antarctic ice sheet is key to sea level rise; current models are inadequate.**

- **ASCR-funded BISICLES ice sheet model built on FASTMath Chombo uses AMR to resolve essential fine scales at ice-ocean interface.**

- **Ongoing collaboration among BISICLES and BER-sponsored IMPACTS, COSIM to couple ice sheet and ocean models**
  - **2011/2012 ALCC (5.5 M Hopper hours)**
  - **Results: POP has been modified to allow dynamic ice shelf interactions.**
  - **Initial 0.1º-resolution standalone _global_ POP runs on Hopper validate the ability to simulate realistic circulation patterns in Antarctic marginal seas.**
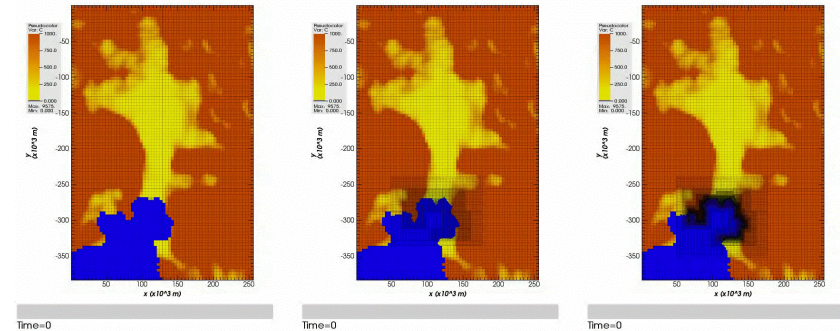
BISICLES Pine Island Glacier simulation showing why mesh resolution is crucial for grounding line behavior.
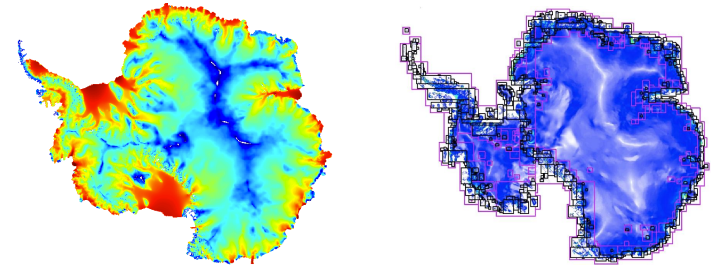
Antarctic ice speed computed using Hopper (left). AMR grid (right) enables < 1-km resolution
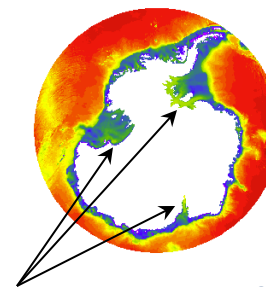
Enhanced Antarctic POP ocean model showing inclusion of regions _under_ ice shelves to allow advection of heat from the ocean to ice right up to the glacier grounding lines.

PI: W. Collins (LBNL)

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- **NERSC and ESnet were vital in the successful measurement of the θ_{13} neutrino transformation.**
  - **Last and most elusive piece of a longstanding puzzle: why neutrinos appear to vanish as they travel**
  - **The answer – a new, surprisingly large type of neutrino oscillation – affords new understanding of fundamental physics; may eventually help solve the riddle of matter-antimatter asymmetry in the universe.**

- **Experiment could not have been done without NERSC: PDSF for simulation and analysis; HPSS and data transfer capabilities; and NGF and Science Gateways for distributing results**
  - **NERSC is the only site where all raw, simulated, and derived data are analyzed and archived.**
  - **=> Investment in experimental physics requires investment in HPC.**

The Daya Bay experiment counts antineutrinos at detectors in three experimental halls (EH) near the Daya Bay nuclear reactor and calculates how many would reach the detectors if there were no oscillation. The plot shows measured disappearance of antineutrinos as a function of distance from the reactor. The 6.0% rate deficit at EH3 provides clear evidence of the new transformation.

NERSC's PDSF cluster   *Daya Bay detectors*

PI: Kam-Biu Luk (LBNL)

HEP

Lawrence Berkeley National Laboratory
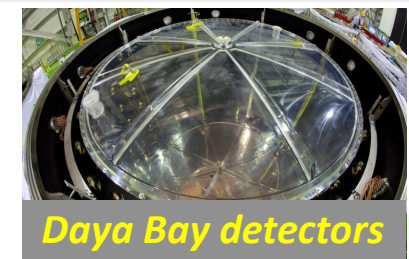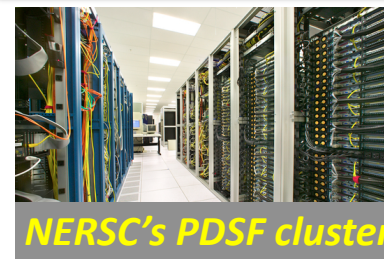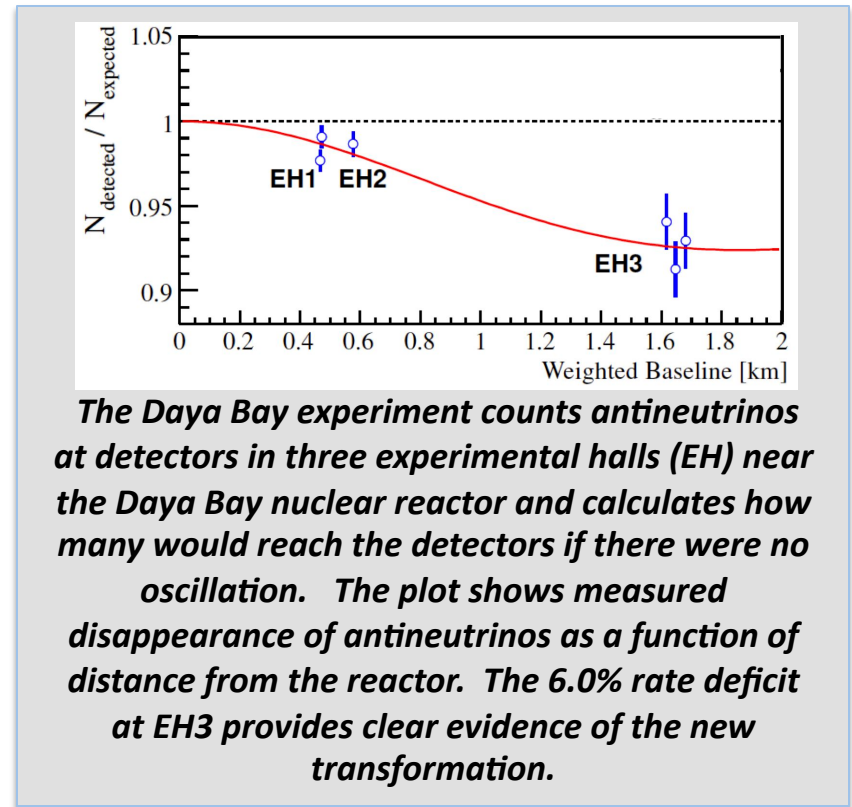
• **The Integrated Microbial Genomes (IMG) system serves as a community resource for comparative analysis of publicly available genomes.**

• **The system crossed the 1 billion gene boundary only last December; now over 3 billion**

• **IMG data integration pipeline and biological interpretation jobs routinely use 20,000 – 75,000 cores on Hopper.**

• **Significant NERSC support in workflow tools, data management tools, and scripting**

• **A metagenomics dataset pipeline at NERSC can process 100 million genes in few days, a task that used to require weeks at the JGI.**

The large computational and storage capacity of NERSC in combination with new analysis techniques ensure sustainability of IMG's integrated-context analysis methods for at least the next two years.

Microbial genome & metagenome analysis

❖ **General aims**
  ▪ Understand microbial life
  ▪ Apply to agriculture, bioremediation, biofuels, human health

❖ **Specific aims include**
  ▪ Predict biochemistry & physiology of organisms based on genome sequence
  ▪ Explain known biochemical & physiological properties
    ☞ Metabolic reconstruction

Radial Phylogenetic Tree

JGI now producing published work with NERSC resources:
Nucl. Acids Res. (2012) 40 (D1): D115-D122.

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**PI: V. Markowitz (LBNL)**

- **Some decades (e.g., 2000–2009), show little increase in observed global temperatures (or even a slight decrease), despite a net positive energy flux into the climate system.**
  Where is the "missing heat" from this influx?

- **Simulations using CCSM have revealed key evidence that this heat is stored in the deep ocean.**

  - **Simulations suggest that these "hiatus periods" are relatively common, will continue to happen, and are one reason why global temperatures do not simply rise in a straight line.**

  - **Hiatus periods are nevertheless consistent with greenhouse-gas-induced warming.**

  - **Study done using computing resources at NERSC, OLCF and NCAR's Climate Simulation Laboratory.**
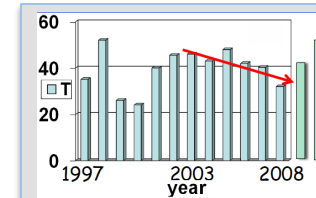
Global average temperatures. 2008 is the coolest year since 2000, despite CO_2 continuing to rise. Where did extra greenhouse heat go in this period?
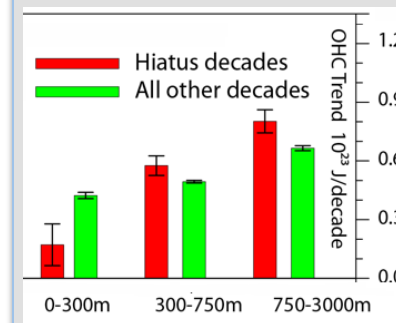
Simulated ocean heat content (OHC) at three depth ranges showing that during hiatus decades (red) more heat is absorbed by deeper waters.
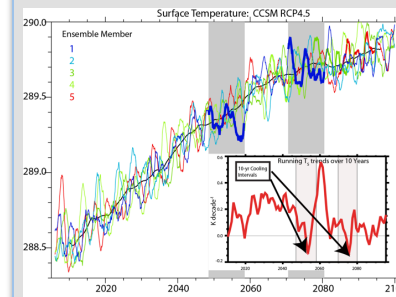
Simulated annual mean surface temperatures 2000 - 2100, highlighting two decades with decreasing mean temperature.

Nature Climate Change Vol 1 Oct 2011

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PI: W. Washington (NCAR)

Designer Piezoelectricity

- **Piezoelectricity: the property of some materials to produce electric charge when bent, squeezed or twisted**
  - Also reversible: piezomaterials change shape when electricity is applied; yields mechanical control
- **Molecular simulations have explained fine-tuning of piezoelectricity in doped graphene.**
  - First example of nanoscale piezoelectricity
  - Used NERSC-provided Quantum ESPRESSO software
- **A fundamentally new form of piezoelectricity *engineered* into a non-piezoelectric material**
  - And a new way to control nanoscale electronics
- **May lead to new devices, from electronics and photonics to energy harvesting, chemical sensing, and high frequency acoustics**
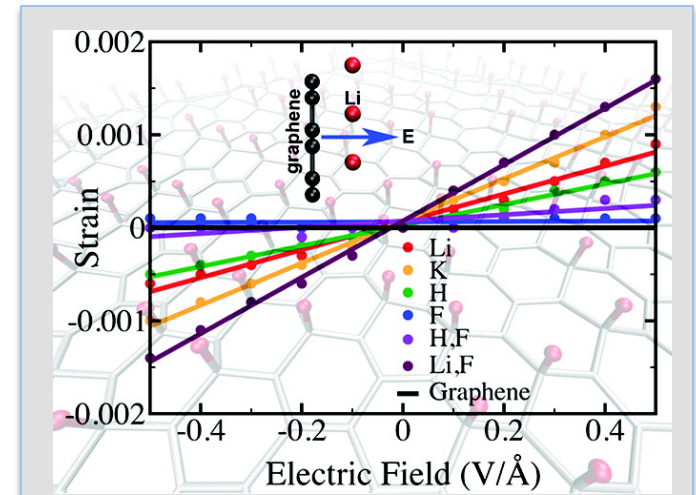

Predicted piezoelectric coefficients (slope of the lines) for graphene and graphene with different atoms added. An electric field applied in the direction of the blue arrow induces a piezoelectric strain that varies with the strength of the field.

ACS Nano December 23, 2011

Important New Method for Studying Solar Materials

- **Goal: develop and use first-principles computational methods to understand, predict, and design novel electronic, optoelectronic, photovoltaic, and thermoelectric materials.**

- **Accomplishment: Using a NERSC NISE award, researchers were able to compute the phonon-assisted interband optical absorption spectrum of silicon entirely from first principles.**

  - **Nearly all commercially-available photovoltaic cells currently depend on this absorption process.**

  - **The new method is general enough to to study fundamental physics of other optoelectronic and photovoltaic materials and can address questions that are not accessible by experiment.**

- **Used the BerkeleyGW software written by new NERSC USG consultant Jack Deslippe.**
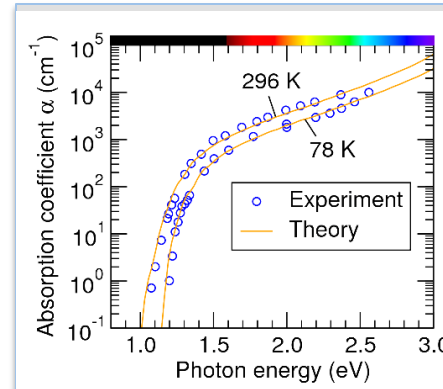
Absorption spectrum of silicon for two temperatures showing excellent agreement between computed and experimental values.

PI: E. Kioupakis (U Michigan)