NERSC Science Highlights

A selection of scientific results produced by NERSC users

December, 2011

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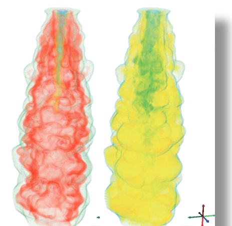
NERSC National Energy Research Scientific Computing Center

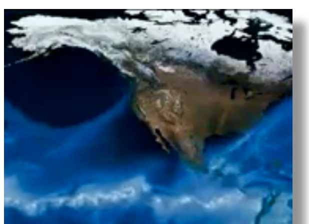
BERKELEY LAB Lawrence Berkeley National Laboratory

NERSC User Scientific Accomplishments, Q4CY2011

Energy
Breakthroughs in battery technologies may extend the range of electric cars.
(D. Mei, PNNL, L-W. Wang, LBNL)

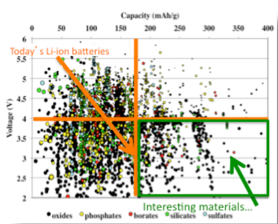
Energy
NERSC resources were used to model a real coal gasifier with a Large Eddy Simulation code.
(P. Smith, U. Utah)





Climate
New techniques help detect extreme events burried in immense data sets.
(Prabhat, M. Wehner, LBNL)

Materials
New screening project already showing impressive results
(Prabhat, M. Wehner, LBNL)



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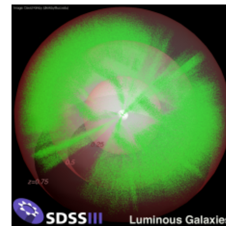
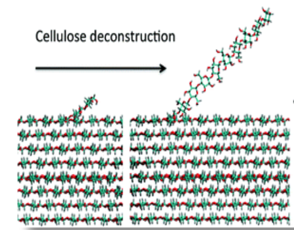
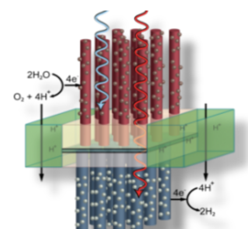


Astrophysics
Clearest pictures of dark matter and biggest 3-D color map of the universe ever constructed
(P. Nugent, LBNL)

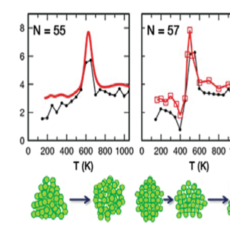
Energy
An unprecedented mechanistic understanding of solvent-induced cellulose deconstruction
(J.-W. Chu, UC Berkeley)





Energy
Simulation is playing a key role in highly visible quest to develop artificial photosynthesis.
(L. Wang, LBNL)

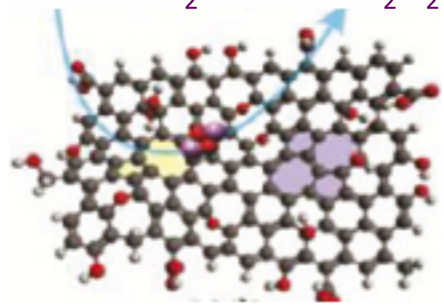
Materials
Computation explains the size-sensitive melting behavior of metal nanoclusters.
(S. Wei, NREL)



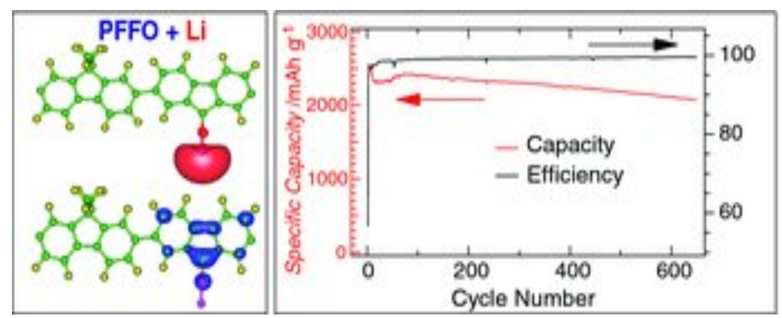
Breakthroughs in Battery Technologies at NERSC

- Computations at NERSC could allow much higher charging capacity, extending the range of electric vehicles.
- Density Functional Theory (DFT) calculations explained the improvement in a new graphene-based lithium-air battery electrode that has the highest charging capacity ever reported.
- A novel low-cost, high-performing material for lithium-ion battery anodes was tailor-made using *ab initio* computations.

$2Li^{+} + O_2 + 2e^{-} \rightarrow Li_2O_2$



Modified graphene lithium-air battery electrode with record-breaking charge capacity, work that was featured on the cover of Chemical and Engineering News.



Electronic structure of a new battery material (left) and a graph showing its ability to maintain its performance after more than 600 charging cycles (right).

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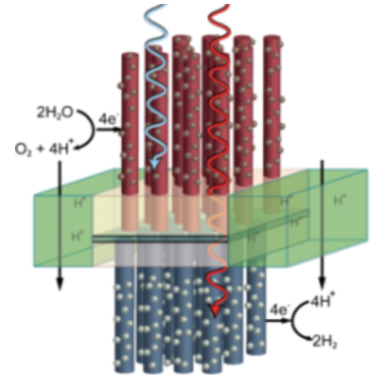
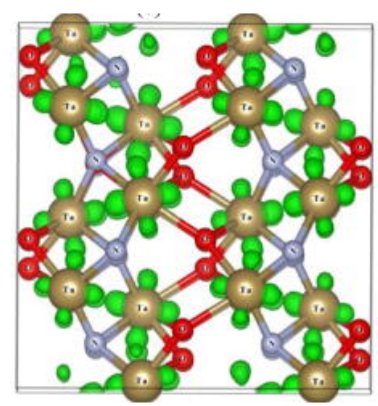
Simulations for Artificial Photosynthesis

DOE's Joint Center for Artificial Photosynthesis Energy Innovation Hub

- JCAP's goal is a photoelectric cell to produce fuel at 10X the efficiency of natural photosynthesis.
  - *"…they're developing a way to turn sunlight and water into fuel for our cars."* - President Obama, State of the Union address, 2011
- 15-year plan to create fuel from sunlight begins with discovery through computation at NERSC.
  - First-principles insight into new light absorbing and catalytic materials via quantum simulations
  - Large scale classical molecular simulations to study nanosized semiconductor quantum rods, critical since nanostructures will be used to split water in JCAP
  - Calculations to identify which materials are stable for photoanodes, a key issue in any practical fuel-from-sunlight solution.



Schematic of a photoelectric cell being designed in a joint LBNL / Caltech effort to harness sunlight for generating chemical fuel.



Early results at NERSC:

Calculations have guided experiments in making new transparent conductors used in photocell design. Work on TaON (left), a new and promising visible-light water splitting material, has been published.

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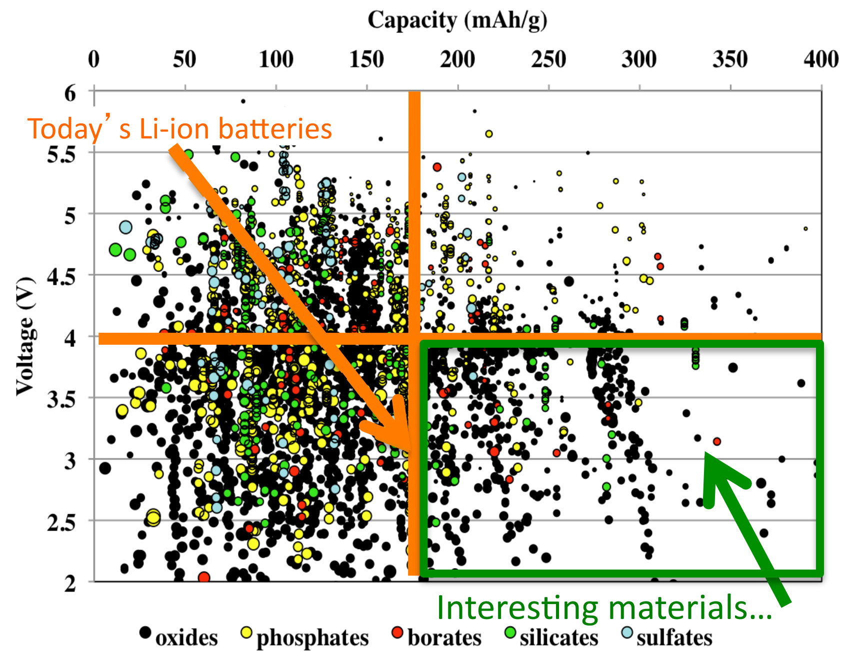
Simulations Speed Materials Discovery

Materials Genome project at MIT / LBNL runs at NERSC

- Invert the materials design problem:
  - I know which properties I want – which materials have those properties?
- Share huge database of simulation results via a web interface
  - Makes HPC results accessible to non-experts
  - Used in academic publications
  - Substantial private sector interest
  - Example: 5,400 materials screened for stable semiconductors that absorb a large part of the solar spectrum; resulted in 15 promising candidates.
- Deep collaboration with NERSC staff
  - Scaling up compute workflow and web applications



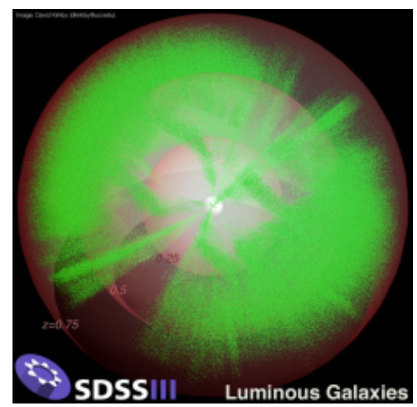
Another example of successful material screening: Ab-initio simulation of over 20,000 potential Lithium-ion battery compounds. The orange area shows materials that are used today or that become unstable; the green area reveals those worth exploring. This research is pushing the boundary of capacity beyond today's limit of 170 mAh/g.

Clearest Pictures Yet of Dark Matter and the Universe

- Tiny distortions in images of distant galaxies are caused by the gravitational influence of dark matter.
  - The most accurate measurements of this "cosmic shear" ever made point the way to better understanding of dark energy.
  - Used the Sloan Digital Sky Survey (SDSS) cosmic image database stored at NERSC

- Other work done at NERSC produced the biggest 3-D color map of the universe ever.
  - Light and color measurements of almost a million galaxies - ranging across the largest volume of space ever used for such measurements – allowed construction of new measurement charts for the universe.

Tiny detail of galaxies from an SDSS image used to plot new maps of dark matter based on the largest direct measurements of cosmic shear to date.



This Luminous Galaxies chart is the biggest 3D map of the universe ever made, covering the period when the universe was only half its present age until now.

Turning Grass Into Gas (For Less)

- Cellulose in biomass can be dissolved by certain ionic liquids but how this happens remains unclear.
- Molecular dynamics simulations have resulted in an unprecedented mechanistic understanding of cellulose deconstruction by ionic liquids.
  - Results show how solvent–sugar interactions change during the deconstruction and which are most important.
  - Variety of systems available at NERSC plays an important role in this work.

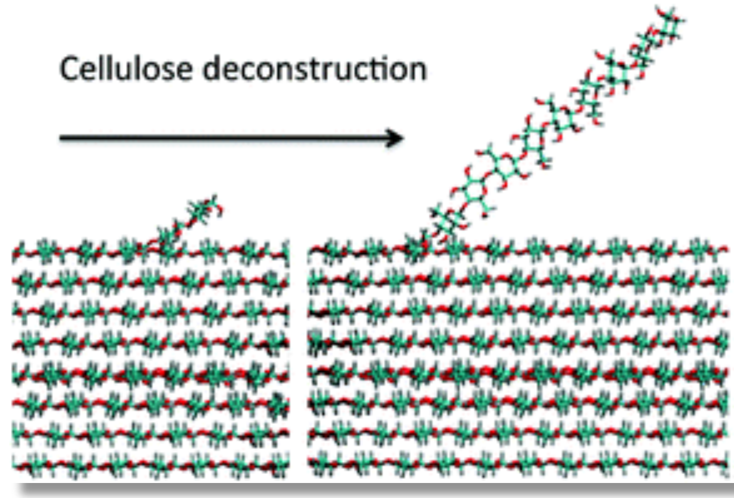


Image showing the simulation in which a strand of cellulose is "peeled" off from the solid cellulose structure. The simulation helped explain the versatility of ionic solvents in attacking a variety of bonds in cellulose.

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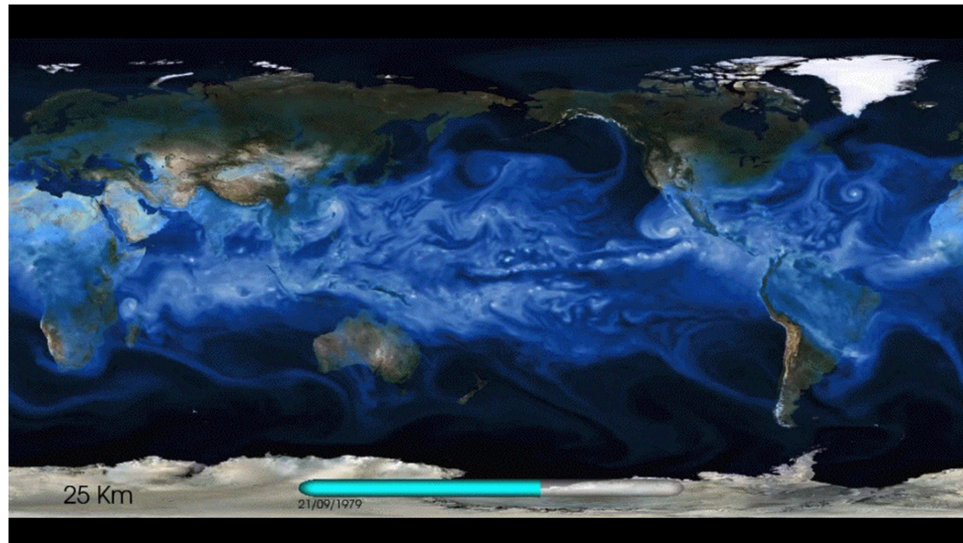
A Better Way to ID Extreme Weather Events in Climate Models

- New state-of-the art data mining, image processing, and topological analysis techniques help detect extreme events, such as hurricanes, that might be burried in
  - 100 TB of output data from a 27-year atmospheric simulation were searched in 2 hours at NERSC.
    - (The Library of Congress contains about 254 TB.)



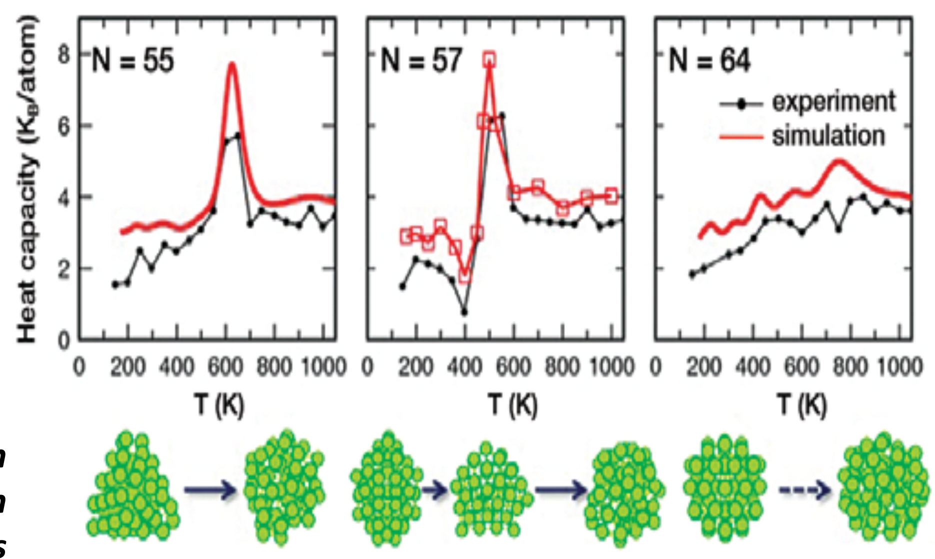
Part of a recent high-resolution atmospheric simulation that was conducted at NERSC.

Computation Reveals Origin of Diverse Melting Behavior in Aluminum Nanoclusters

- Unlike bulk materials, metallic nanoclusters (with about 55 atoms) exhibit size-sensitive melting changes: adding just a *single atom* to a nanocluster can cause a dramatic change in melting behavior. Why?

- Molecular dynamics studies at NERSC by NREL scientists revealed the key role of cluster symmetry on the size-sensitive melting behavior.

- **Key Result** Provides insight for understanding phase changes of nanoparticles, important for thermal energy storage and catalysis.



Simulated heat capacities (red) are compared with experimental data (black) for aluminum nanoclusters consisting of 55, 57, and 64 atoms (shown in green).

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BES – ALCC Project

PI: Suhai Wei (NREL)

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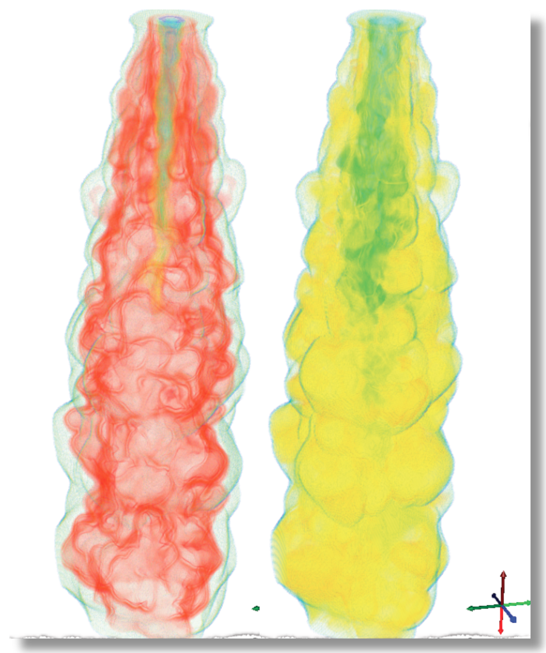
Quantitative Assessment of a Coal Gasification Model

- Coal Gasification offers a versatile and clean method for converting coal into gaseous fuel.
  - But simulation of such a complex physical phenomenon requires significant validation efforts.
- NERSC resources were used to model a real coal gasifier with the ARCHES Large Eddy Simulation (LES) code. LES is required for accurate combustion simulation.
- The validated method can now be used to assess retrofit techniques for coal gasifiers, helping to reduce CO_2 emissions.
- NERSC resources were a vital part of Ph.D. thesis of C.M. Reid, now a postdoc at LLNL.



Influence of coal particle size on temperature: larger particles (right) take longer to heat up

BER – ALCC Project

PI: Philip Smith (University of Utah) *Dec2011*