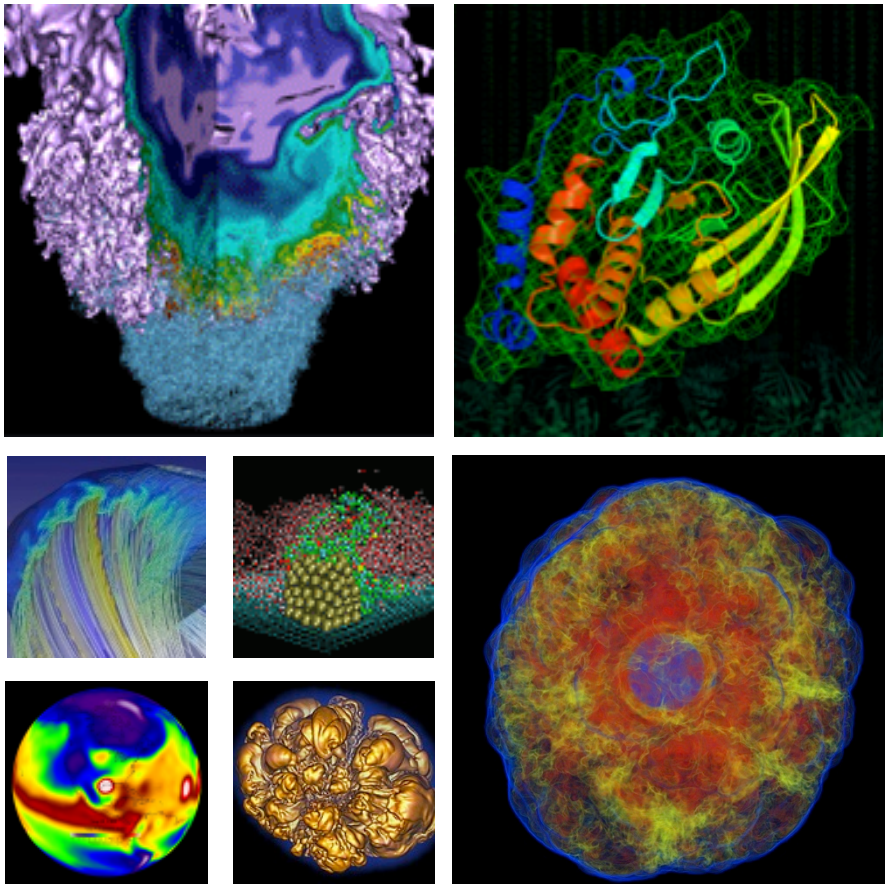
NERSC Science Highlights



Richard Gerber
NERSC Senior Science Advisor

Thanks to Harvey Wasserman

NERSC: Science First

NERSC's mission is to accelerate scientific discovery at the DOE Office of Science through high performance computing and data analysis.

#1 Goal: Scientific Productivity

Systems and Services Designed for Science

How do we know what scientists want and need?

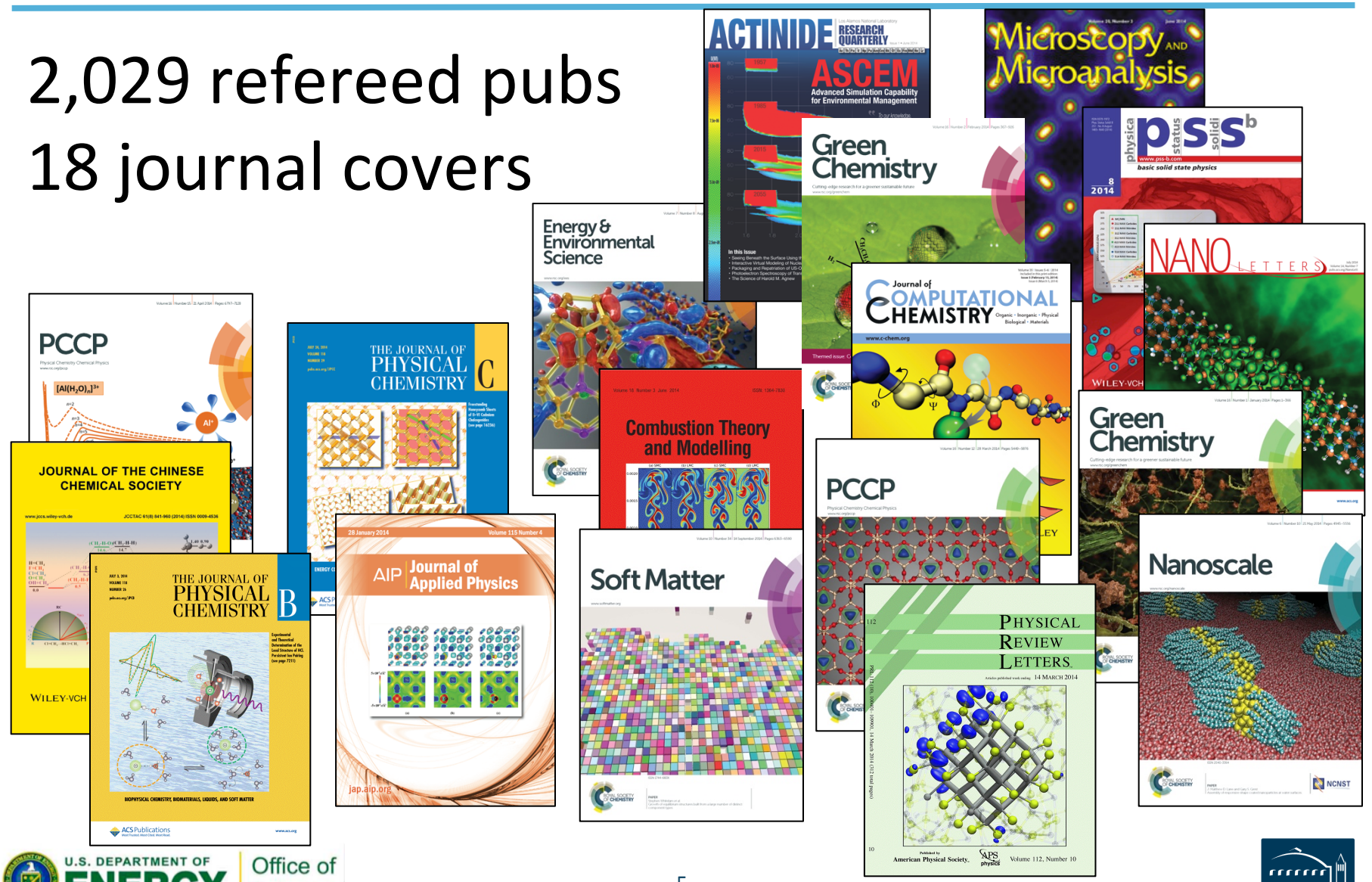
- Requirements Reviews
- NERSC User Group
- Annual User Survey
- ERCAP Allocations Proposals
- Workload Analyses
- Conferences & Workshops
- NESAP Engagements

NERSC is the most scientifically productive Supercomputer Center in the World!

2014 Science Output

2,029 refereed pubs

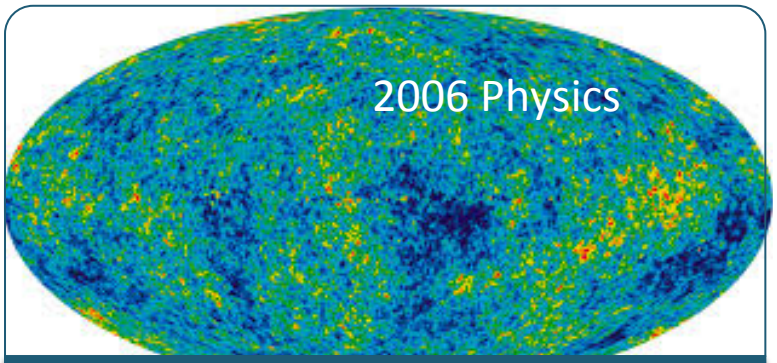
18 journal covers



NERSC Nobel Prize Winners

Martin Karplus

Saul Perlmutter



George Smoot

Warren Washington

In 2014 scientists at NERSC

used

384,000 core-years

3,366,252,235

MPP hours of compute time

and permanently stored

11 million DVDs

54,000,000,000

Mbytes of data

Compute Hours

Edison

1,030 M x 2 =

2,060 M hours

Hopper

1,186 M x 1 =

1,186 M hours

Carver

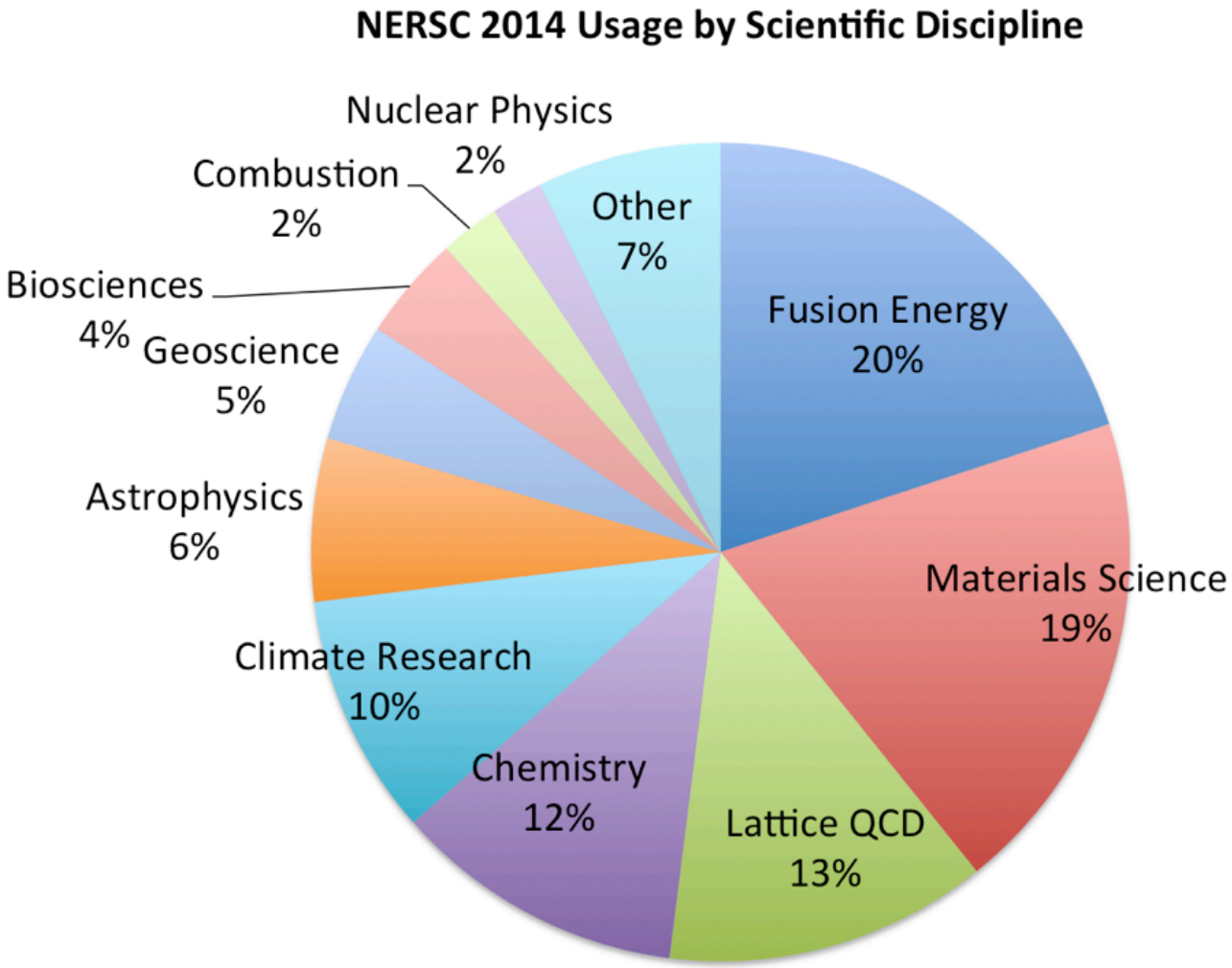
63 M x 1.5 = 95 M hours

Permanent Data Storage

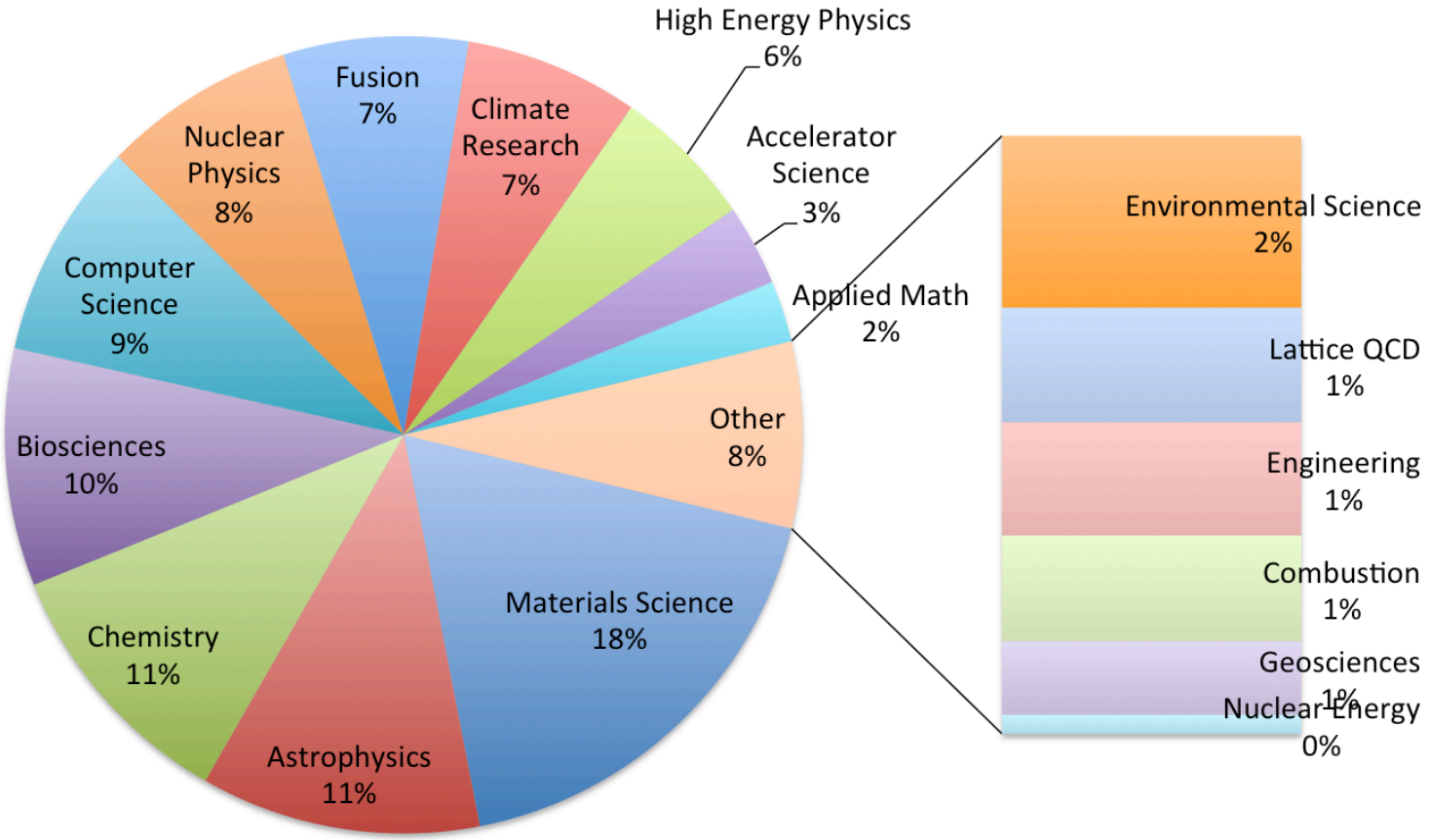
HPSS
50 Petabytes

Project
4 Petabytes

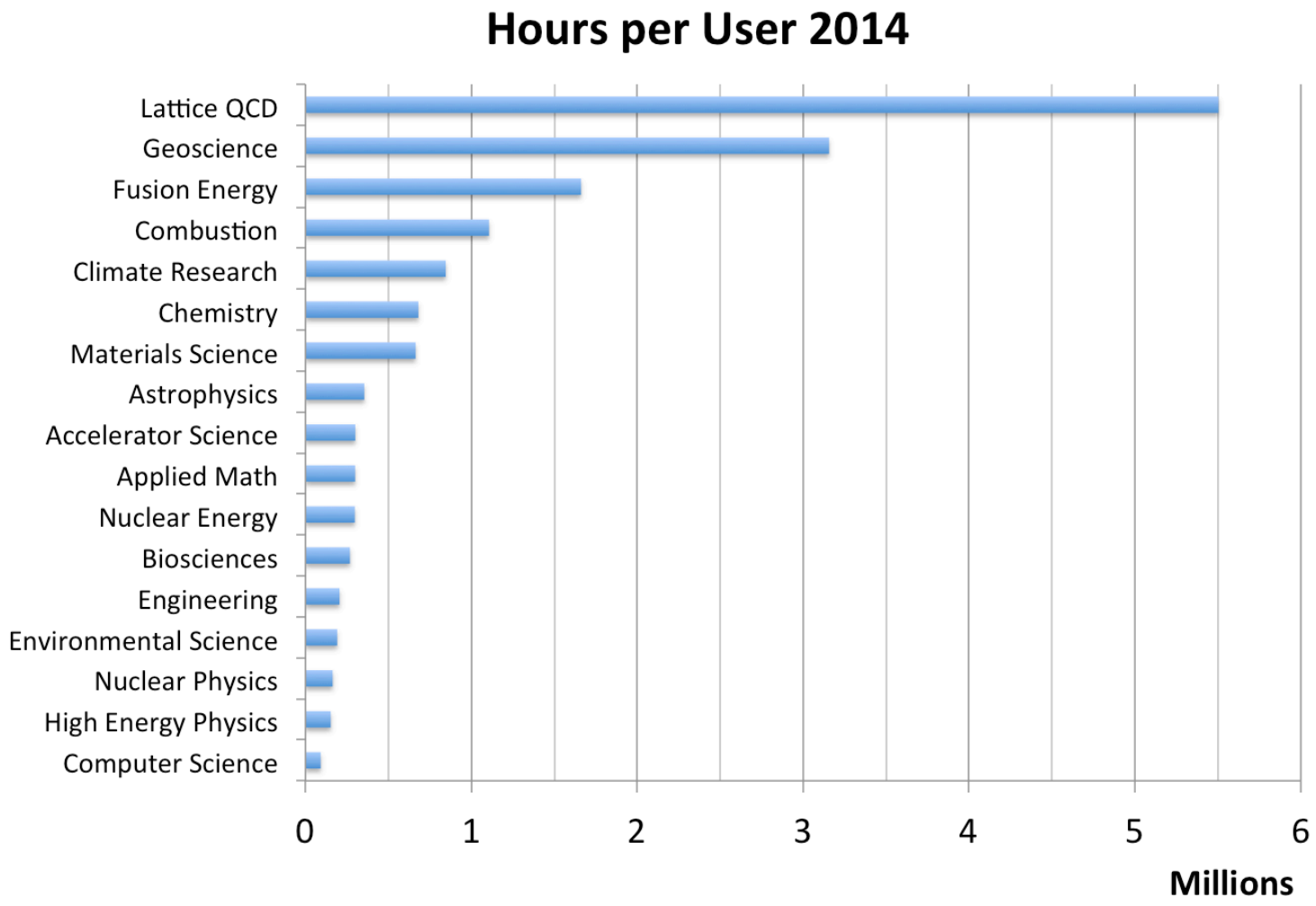
MPP Usage by Science Area



Number of Users by Science Area



Hours per User by Science Area



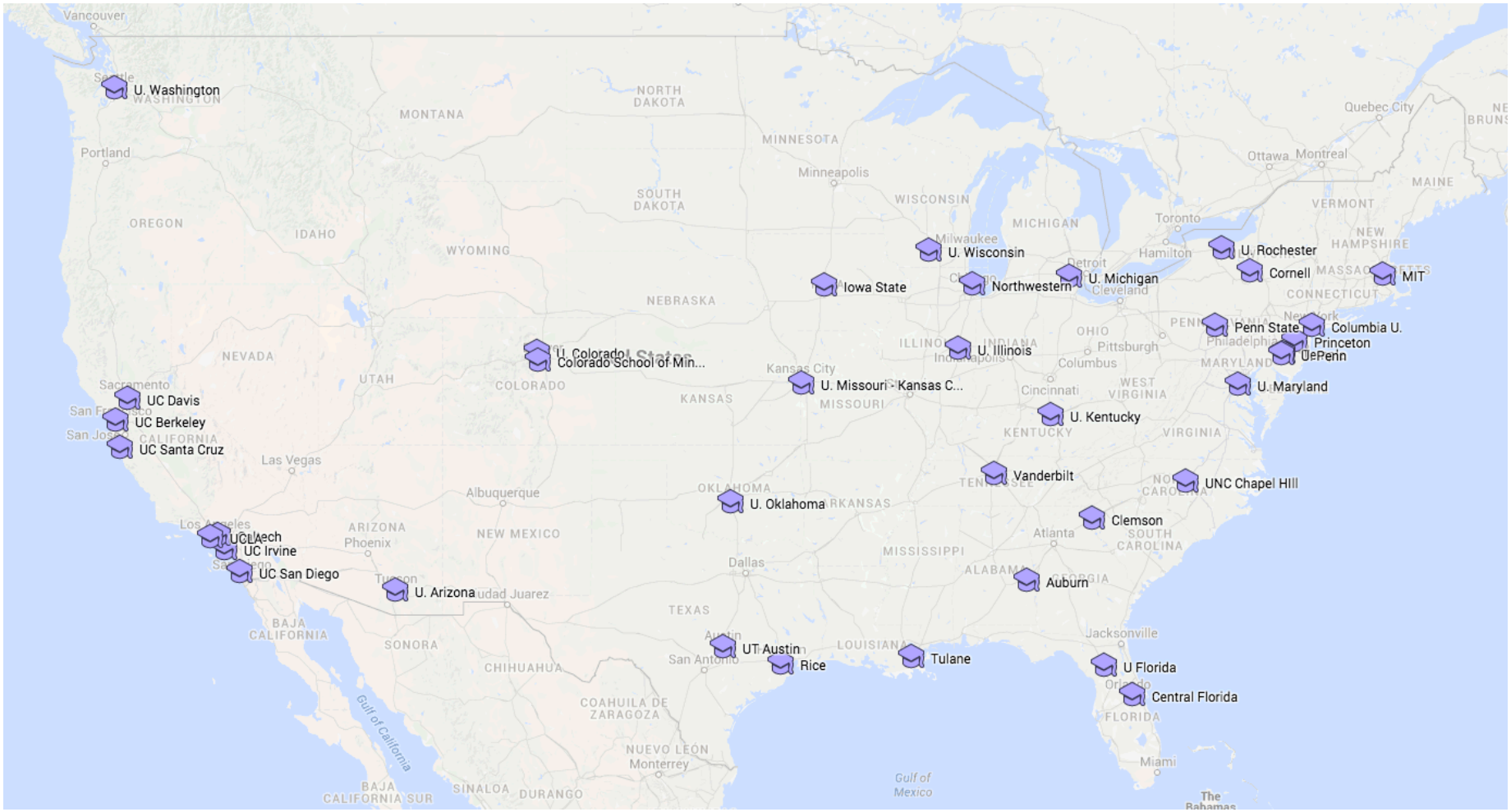
Top Users 2014

User	Org.	Project	Science Field	MPP Hours
Nathan Howard	MIT	Ion and Electron Scale Turbulence in Tokamak Plasmas	Fusion Energy	126 M
Doug Toussaint	U. Arizona	Quantum Chromodynamics with four flavors of dynamical quarks	Lattice QCD	87 M
Petr Petrov	Berkeley Lab	Large Scale 3D Geophyscial Inversion & Imaging	Geoscience	60 M
Karl Hammond	U. Tennessee	PSI SciDAC: Bridging from the Surface to the Micron Frontier	Fusion Energy	56 M
David Trebotich	Berkeley Lab	Subsurface Flow and Reactive Transport Processes Associated with Carbon Sequestration	Geoscience	54 M

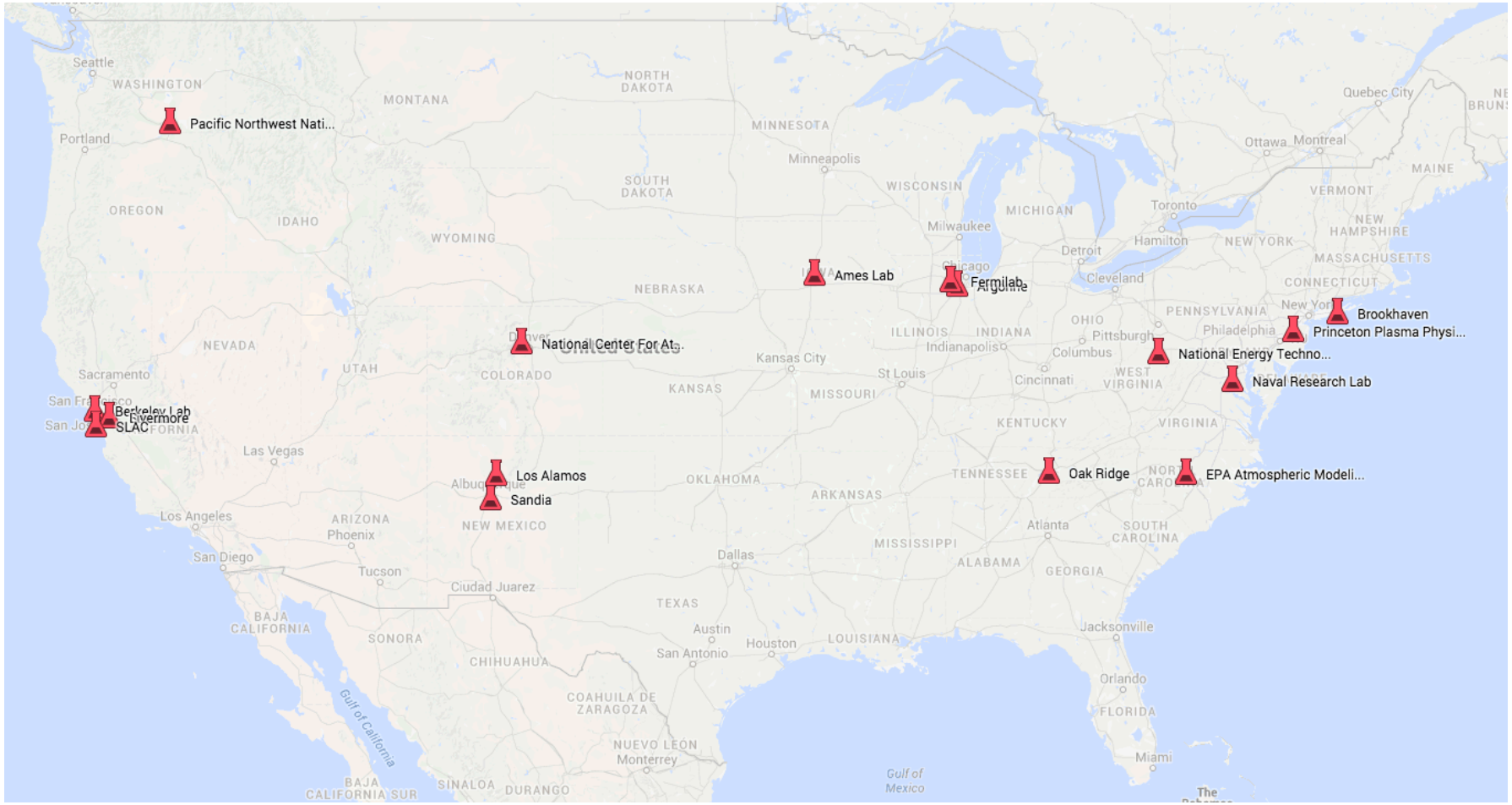
Top Projects 2014

Project	Science Field	PI	Affiliation	MPP Hours
Quantum Chromodynamics with four flavors of dynamical quarks	Lattice QCD	Doug Toussaint	U. Arizona	110 M
Center for Edge Physics Simulation: SciDAC-3 Center	Fusion	C.S. Chang	Princeton Plasma Physics Lab	107 M
Ion and Electron Scale Turbulence in Tokamak Plasmas	Fusion	Chris Holland	UC San Diego	82 M
Lattice QCD Study of the Structure of Light Nuclei	Lattice QCD	Martin Savage	U. Washington	75 M
Exploration of Hadron Structure using Lattice QCD	Lattice QCD	John Negele	MIT	65 M

Top Universities – 60% of usage



Top Labs & Government Agencies



Some of My Favorite Science Stories 2014

Three you'll hear about today:

- **9:30** *Efficient modeling of laser-plasma accelerators*, Carlo Benedetti, BELLA Center and the L'OASIS Program, Berkeley Lab
- **11:15** *Transforming Beamline Science with SPOT Suite*, Craig Tull, Berkeley Lab
- **1:30** *The First Cosmic Explosions - Simulating the First Supernovae with NERSC Supercomputers*, Ken Chen, UC Santa Cruz

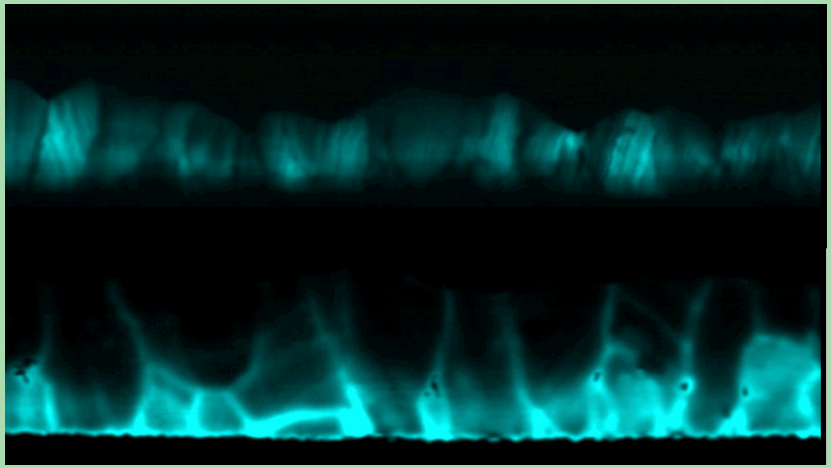
Cheap, Efficient Thin Film Solar Cells

Researchers have made a discovery that could lead to less expensive, more easily fabricated thin-film solar cells.

Experimental fact: Doping Cadmium-telluride (CdTe) solar cells with cadmium-chloride ($CdCl_2$) improves efficiency.

How does this happen?: Previously unknown.

Experiment + Modeling → Chlorine replaces tellurium at grain boundaries



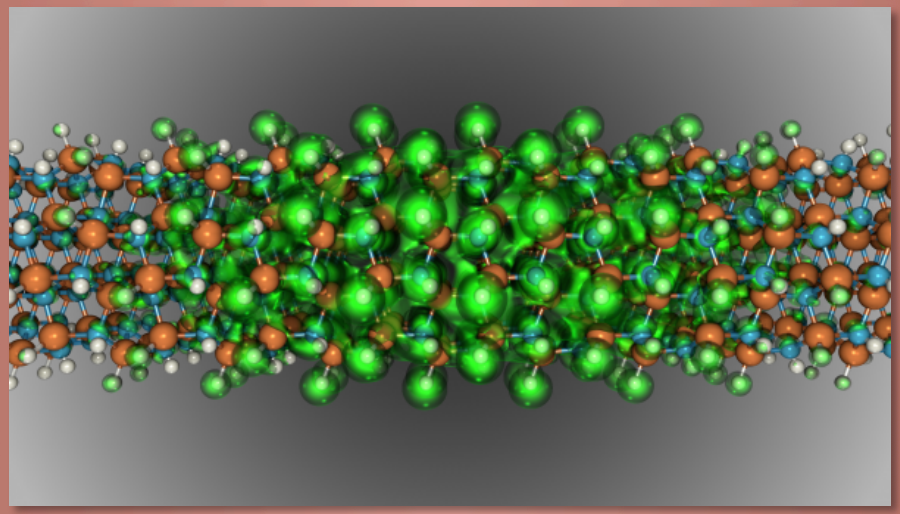
Cross-sectional electron beam-induced current maps show the difference in CdTe solar cells before (above) and after (below) ($CdCl_2$) treatment. The increased brightness after treatment indicates higher current collection at the grain boundaries.

Thin-film CdTe solar cells are considered a rival to current silicon-based systems because of ease of fabrication, but their efficiency has lagged. New results pave the way to designing better materials.

Lead Researcher: Yanfa Yan, University of Toledo
System: Hopper Cray XE6

Phys. Rev. Lett. 112, 156103, April 2014

Brighter, Efficient, Realistic-Looking LEDs



This simulation of a 1 nanometer-wide indium nitride wire shows the distribution of an electron around a positively charged "hole." Researchers found that strong quantum confinement in these small nanostructures enables efficient light emission at visible wavelengths.

Lead Researcher: Emmanouil Kioupakis, University of Michigan
Systems: Edison Cray XC30, Hopper Cray XE6

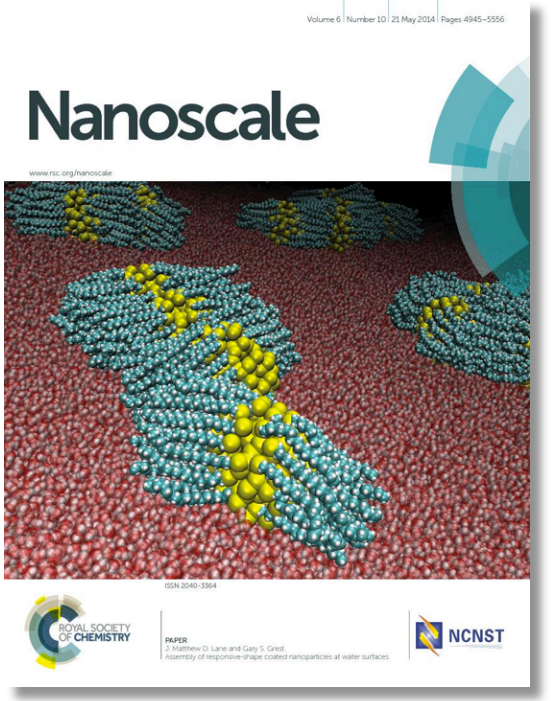
Scientists using NERSC supercomputers have discovered that tiny, atomic-size wires can be used to efficiently produce light that is brighter and more natural-looking than currently used LEDs.

New nanomaterials offer the tantalizing prospect of LEDs that can be "grown" in arrays of nanowires, resulting in lighting that can be thin, flexible, high-resolution, and also very efficient.

Nano Lett., 2014, 14 (7), pp 3709–3714

Controlling NanoParticle Assembly

- Soft materials consisting of polymer-coated nanoparticles (NP) can be used for photonics, filtration, photovoltaics, and other important applications.
- Left to themselves, however, nanoparticles tend to aggregate into useless clumps.
- Scientists have discovered that applying a coating of short-chain polymers can prevent this aggregation
- Using supercomputers at NERSC scientists have found that surprisingly simple short chain polymer coatings can be effectively used to selectively control the aggregation of very small nanoparticles.



Astage in a typical merger of a nanoparticle on one end to an existing cluster. The coating shape dictates a preferred linear arrangement of nanoparticles in aggregates.

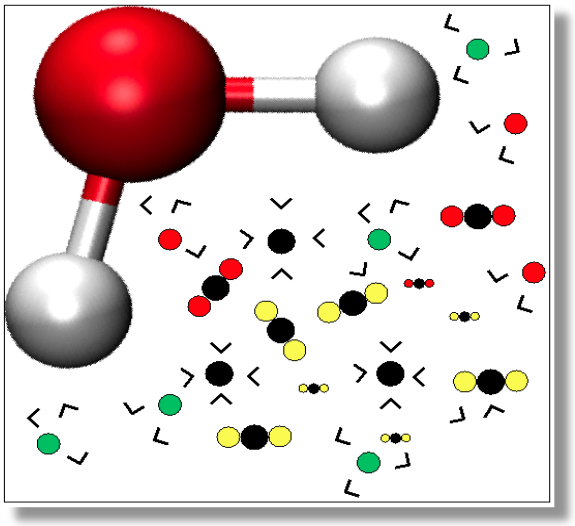
U.S. DEPARTMENT OF ENERGY | Office of Science BES

PI: G. Grest (SNL)

Nanoscale, 2014, 6, 5132

BERKELEY LAB

Understanding the Chemistry of Mercury, a Toxic Pollutant



Artist's conception of how water molecules (black "v" shapes) affect bonding in a variety of molecules containing Hg (red) and other atoms, such as S, O, Se, F, Br, and Cl.

Supercomputer simulations discover how mercury binds preferentially to sulfur-containing molecules.

An interaction between mercury and water molecules is important to the process, a finding that is impossible from experimentation alone.

These results are needed to understand the toxicity and environmental fate of mercury, a major global pollutant.

Lead Researcher: Jeremy Smith, Oak Ridge National Laboratory
Systems: Hopper Cray XE6

J. Phys. Chem. Lett., 2013, 4 (14), 2317

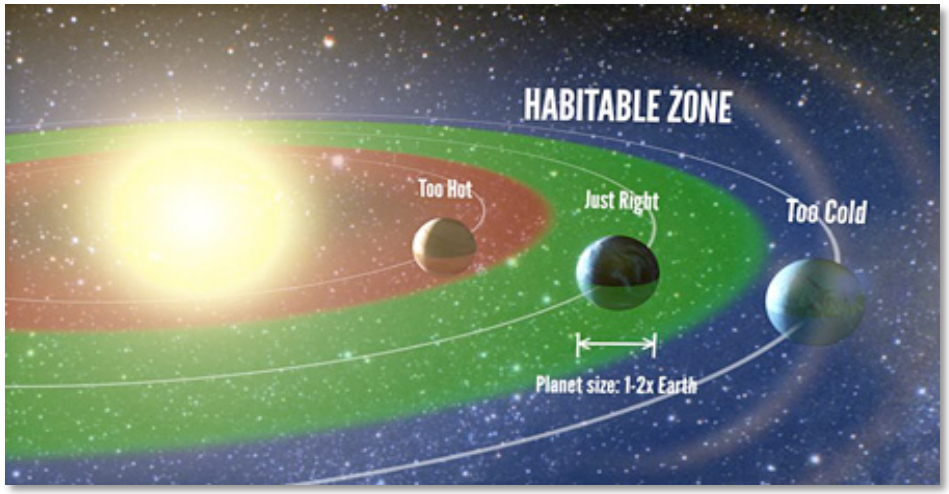
Billions of Potentially Habitable Planets

Are Earth's rare?

No! Our galaxy may hold up to 40 billion habitable planets, some possibly around stars near enough to be seen with the naked eye.

Researchers used NERSC supercomputers and software pipeline to analyze 4 years of Kepler Satellite data.

Lead Researcher: Erik Petigura, UC Berkeley
Systems: NERSC data systems, Carver



Artist's representation of the "habitable zone," the range of orbits where water can exist as a liquid on the surface of a planet.

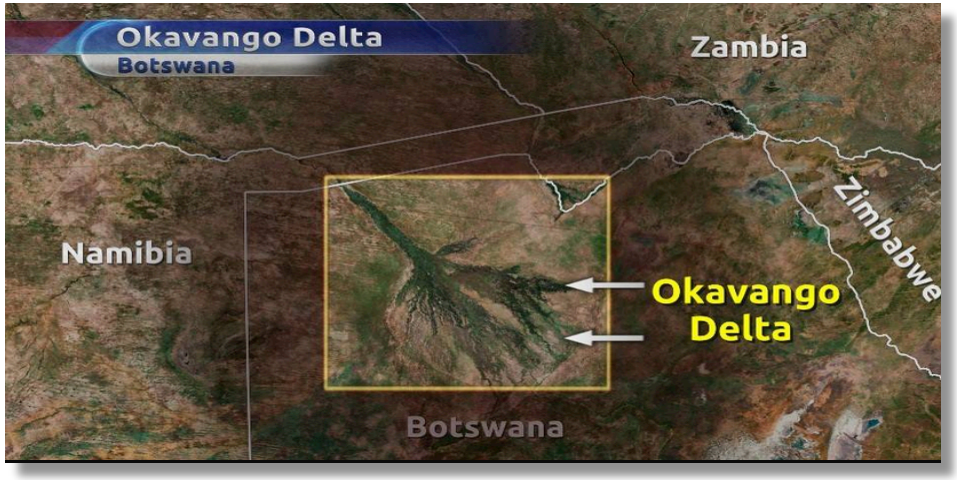
100,000 stars analyzed for dimming caused by planets blocking some of star's light

Required 10 billion sets of calculations per star

Proc. National Acad. of Sciences, 2013, vol. 110 no. 48

Unexpected Climate Modeling Result: Decreased Flooding From Higher Temps

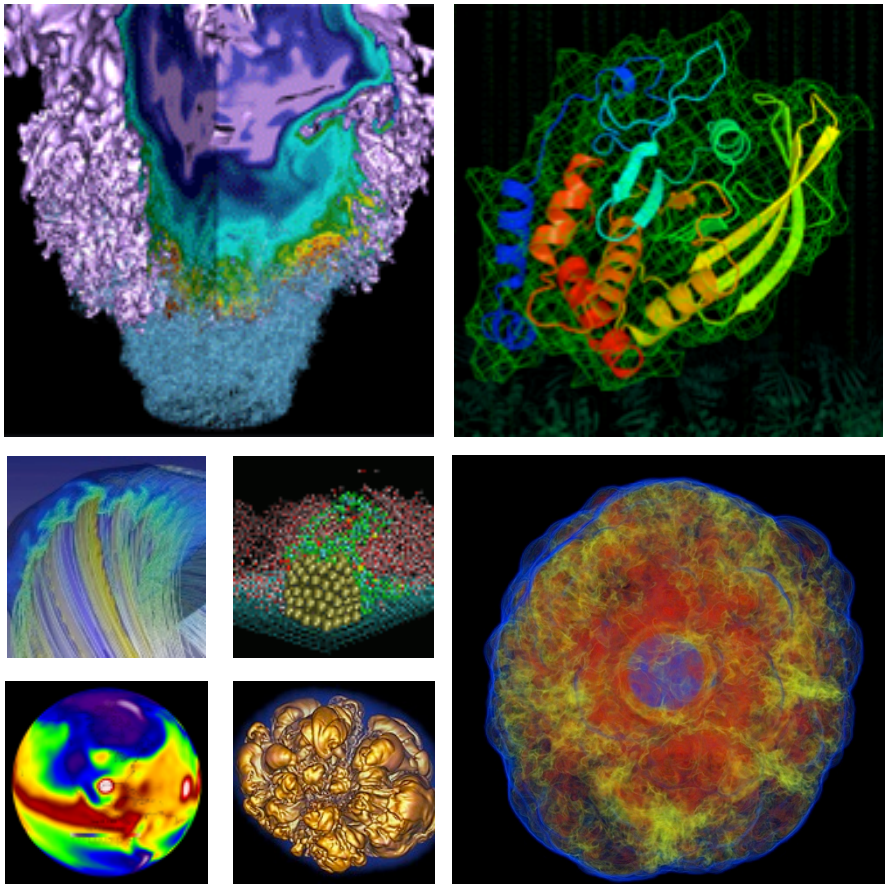
- Greenhouse gas-caused climate change *reduces* chances of flooding in the Okavango River Basin in southern Africa.
- Warmer air leads to more evaporation from the slow-moving river while causing little change in rainfall in the region.
- The huge floods of 2009-2011 would apparently have been much *worse* without the current warmer climate.



The inset shows the region subjected to intense flooding in recent years. Climate simulations done at NERSC strongly suggest that this flooding is not a result of greenhouse gas-induced climate change.

Journal of Hydrology 511 (2014) 350–358

ERCAP Quiz: Science or Fiction*



Richard Gerber

NERSC Senior Science Advisor

February 25, 2015

*Idea blatantly stolen from numerous sources.

I'll show you four brief project descriptions from this year's ERCAP submissions.

Three are real and one is fiction.

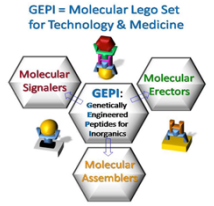
Your job is to identify the fiction.

If you know the answer, don't shout it out!

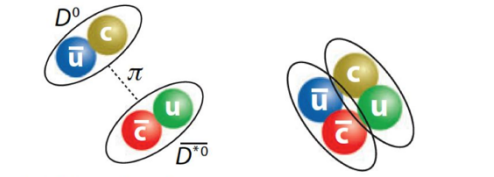
Vote with your applause after you've seen all four.

ERCAP Science or Fiction?

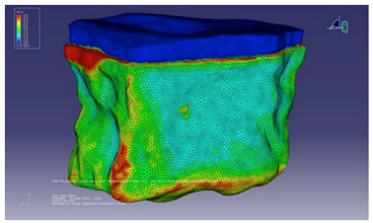
Investigation of Self-Assembled Peptide-Enabled Hybrid Two Dimensional Nanodevices



Investigation of Exotic Charmonium States



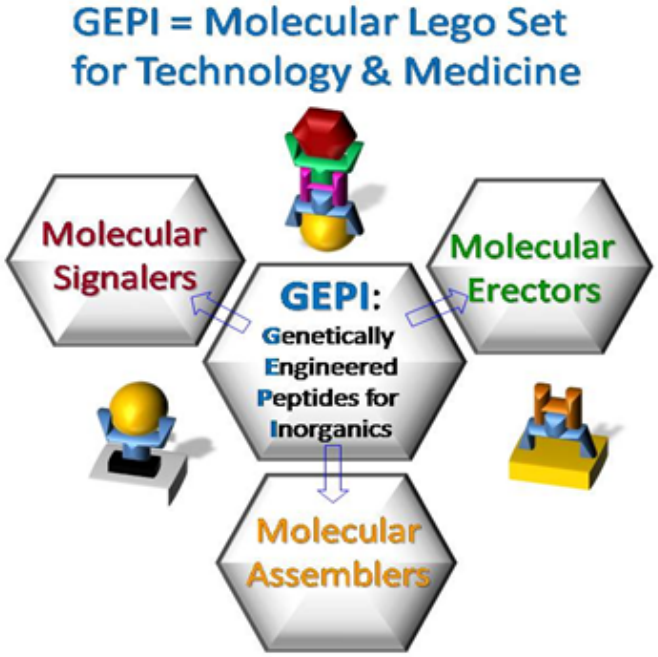
High Resolution Model Development to Quantify the Impact of Melting Icebergs on Global Sea Levels



Advancing Computing Performance of EnergyPlus by Two Orders of Magnitude

Self-Assembled peptide-enabled hybrid two dimensional nanodevices Science!

- Proteins are the workhorses of biology
- This project selects and tailors peptides with desired inorganic-binding and assembly properties that were never intended by nature …
- And uses them as molecular building blocks in practical applications, from materialization, to molecular medicine, and energy systems.



Prof. Dr. Mehmet Sarikaya,
University of Washington

Investigation of exotic charmonium states

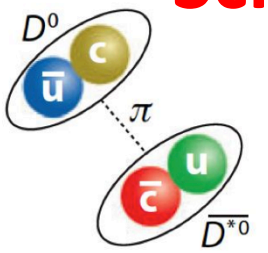
Experimental measurements have discovered excited states of charmonium that cannot be explained by the conventional quark model.

Particle X(3872) has a mass of 3871.2 MeV/c^2, but what is it?

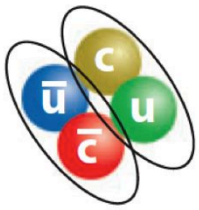
It could be a tetraquark: a particle consisting of four quarks.

It could also be a "molecule" of D0 and anti-D0 mesons. (A D0 is a charm and an anti-up quark.)

Science!



D^0–$\overline{D^{*0}}$ "molecule"



Diquark–diantiquark

These two particles would be bound together just like two hydrogen atoms can bind together to make a gaseous hydrogen molecule.

Paul Mackenzie, FNAL

Advancing computing performance of EnergyPlus by two orders of magnitude

EnergyPlus is the U.S. DOE's flagship whole-building energy simulation engine.

Science!

EnergyPlus takes input a building's geometry, construction materials, HVAC systems, operations and control schemes, occupancy schedules, and prevailing weather conditions and calculates the energy and water used to maintain occupant comfort.

The goal is to reduce EnergyPlus execution time by two orders of magnitude or more.

The team wants to improve parallel simulation algorithms to take advantage of Cori.

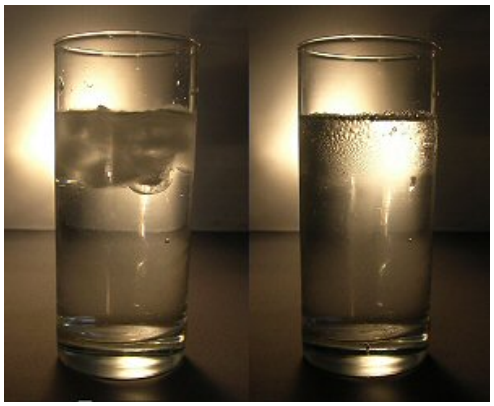
Sang Hoon Lee,
Yixing Chen, LBNL

High resolution model development to quantify the impact of iceberg melting on global sea levels

Fiction!

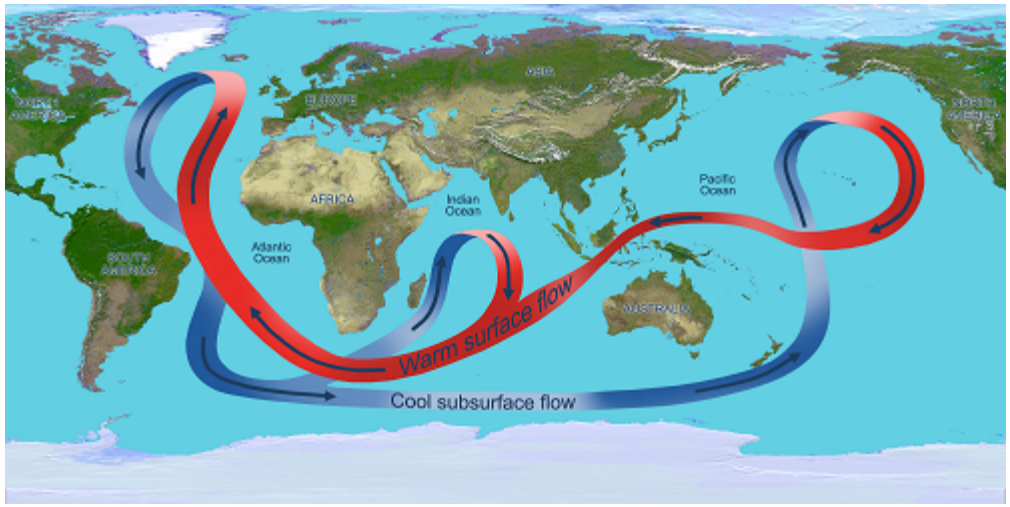
An object that floats displaces the amount of water that has the same weight as the object.

Melting icebergs don't change sea level.



Science!

High resolution model development to quantify the impact of iceberg melting on the stability of the Atlantic Meridional Overturning Circulation



Alan Caldron, U. Mass.

National Energy Research Scientific Computing Center

Section Title