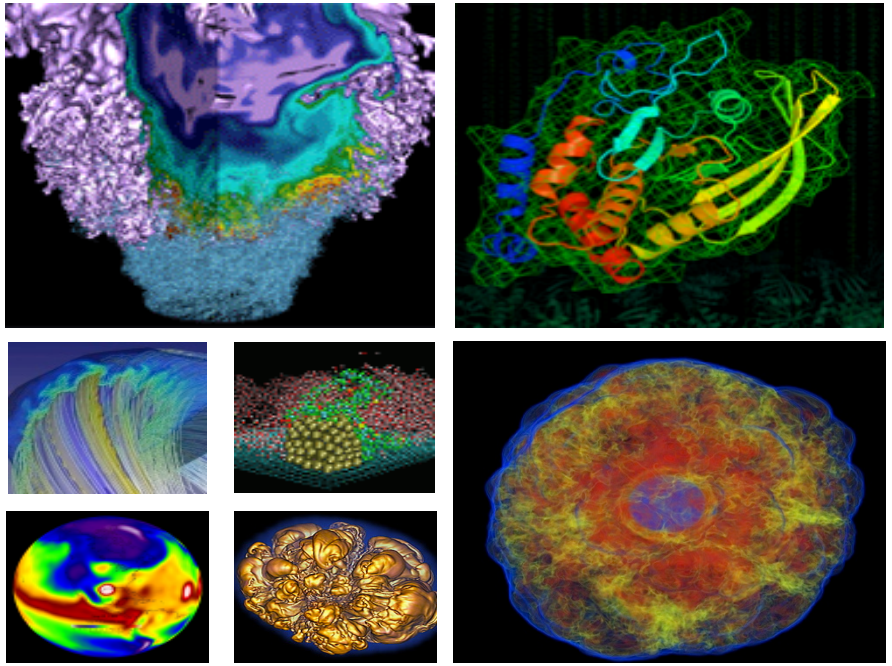
High Performance Computing and NERSC



Richard Gerber

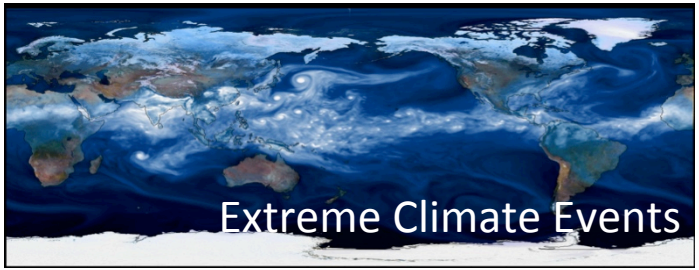
Senior Science Advisor

HPC Department Head

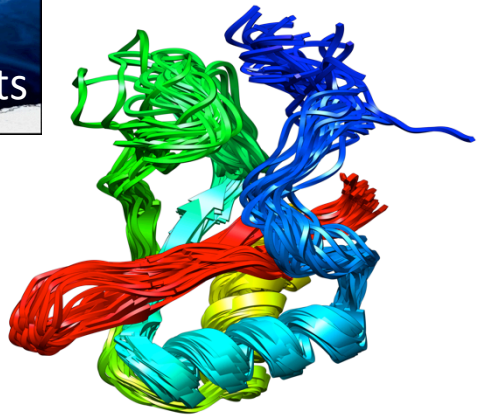
February 27, 2017

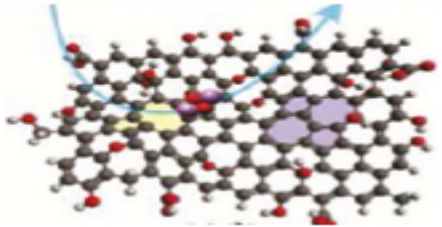
High Performance Computing is …

… the application of "supercomputers" to scientific computational problems that are either too large for standard computers or would take them too long.



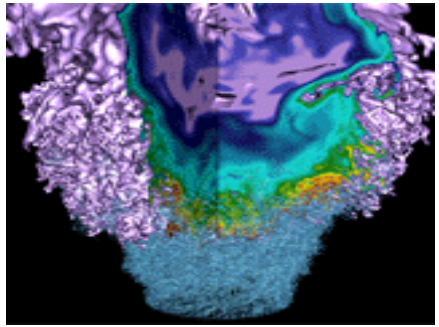
Understanding How Proteins Work



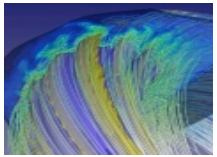


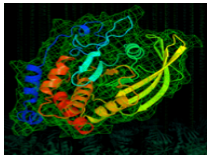
Designing Better Batteries

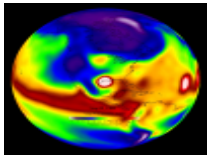
What is a Supercomputer?

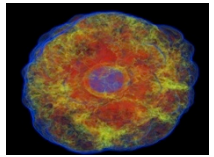


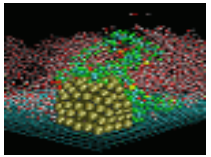
NERSC











What is a supercomputer?

A. A computer with a CPU vastly more powerful than the one in my laptop or phone.

B. A quantum device that takes advantage of the fact that entangled quantum particles can simultaneously exist in a many states.

C. Processors not so different than the one in my laptop, but 100s of thousands of them working together to solve a problem. ✔

A Supercomputer is …

… not so different from a super high-end desktop computer.

Or rather, a lot of super high-end desktop computers.

Edison, show above, has 5,576 “nodes” (~a powerful desktop), each with 24 compute cores for a total of

133,824 compute cores
~2×10^{15} calculations/second

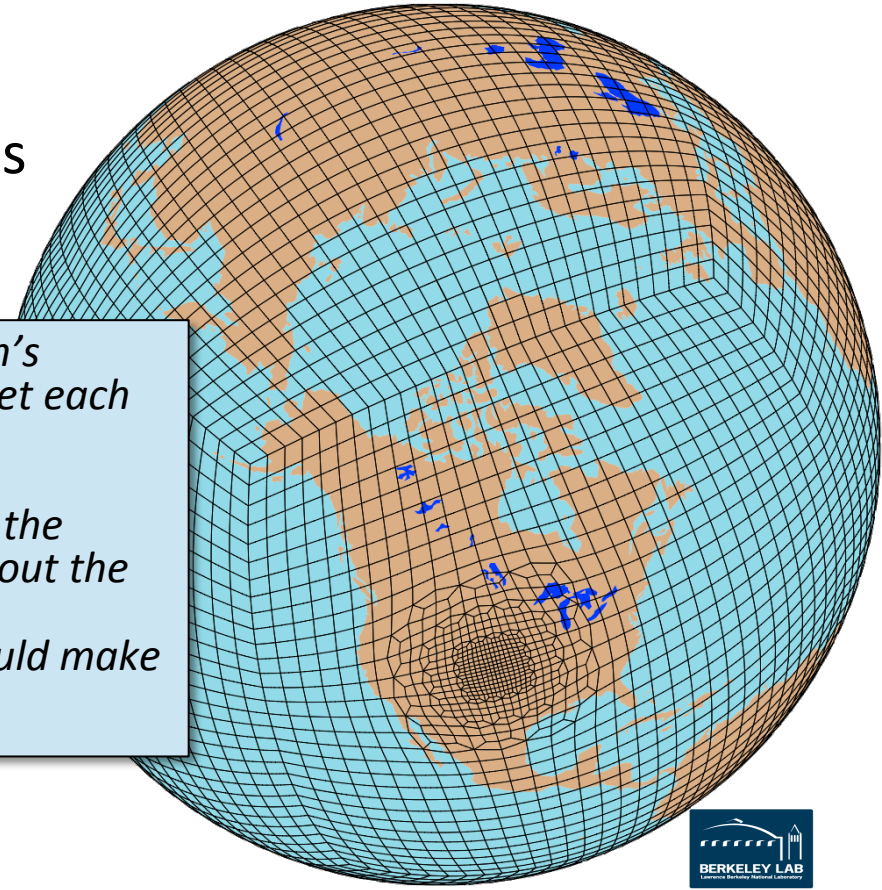
7 billion people
on 3 million Earths
doing 1 calculation
each second
= 1 Edison

Parallel Computing on Supercomputers

- In parallel computing, scientists divide a big task into smaller ones
- "Divide and conquer"

For example, to simulate the behavior of Earth's atmosphere, you can divide it into zones and let each processor calculate what happens in each.

From time to time each processor has to send the results of its calculation to its neighbors. Without the high-speed custom network available on supercomputers, this communication step would make the calculations take much too long.



Custom Powerful Network

The nodes are all connected to each other with a high speed, low latency network.

This is what allows the nodes to "talk" to each other and ***work together to solve problems*** you could never solve on your laptop or even 150,000 laptops.

Typical point-to-point bandwidth

Supercomputer: 10 GBytes/sec
Your home: 0.02* GBytes/sec

5,000 X

Latency

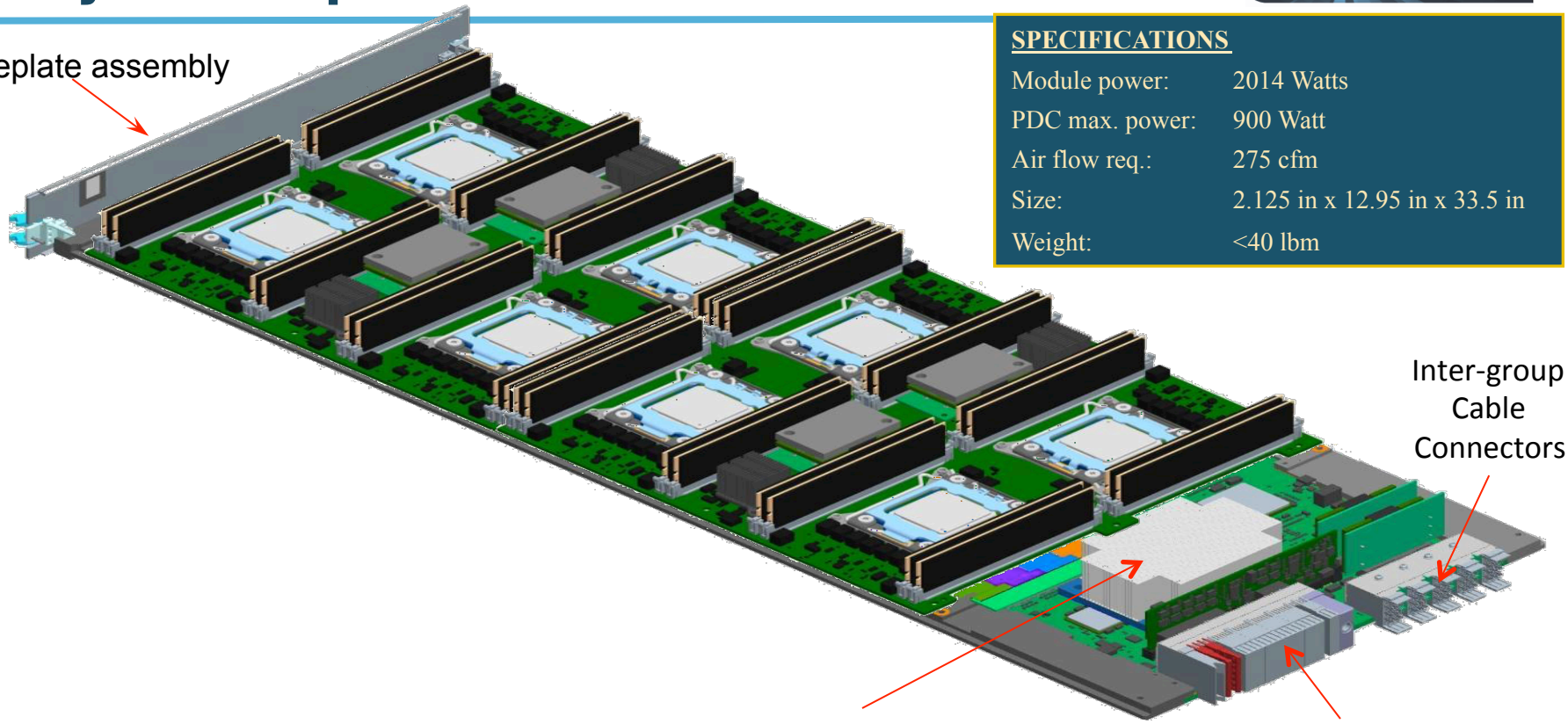
Supercomputer: 1 µs
Your home computer: 20,000* µs

20,000 X

Cloud systems have slower networks

* If you're really lucky

Cray XC Compute Blade



SPECIFICATIONS

Module power:	2014 Watts
PDC max. power:	900 Watt
Air flow req.:	275 cfm
Size:	2.125 in x 12.95 in x 33.5 in
Weight:	<40 lbm

Data

How big is 26 PBs?

338 years of HD video

½ the entire written works of mankind ever, in all languages

PBs of fast storage for files and data

Cori: 26 PB
Your laptop: 0.0005 PB
Your iPhone: 0.00005 PB

45,000 X

Cloud systems have slower I/O and less permanent storage

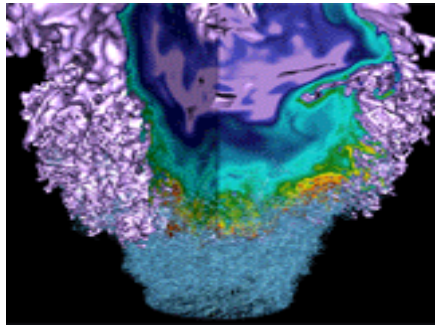
Write data to permanent storage

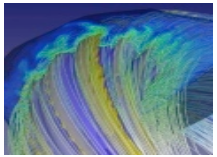
Edison: 140 GB/sec
My iMac: 0.01 GB/sec

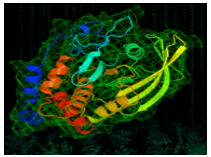
14,000 X

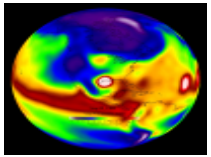
HPSS tape library:
75 PB

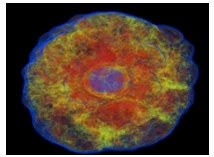
What is NERSC?

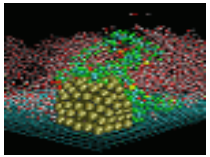












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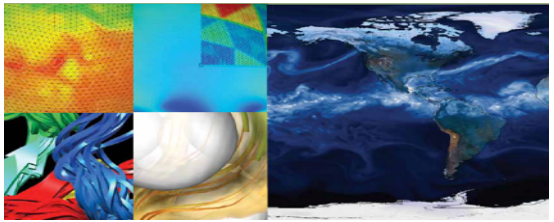
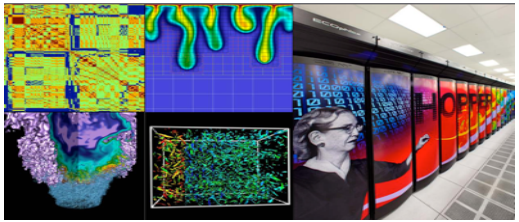
U.S. DEPARTMENT OF ENERGY | Office of Science

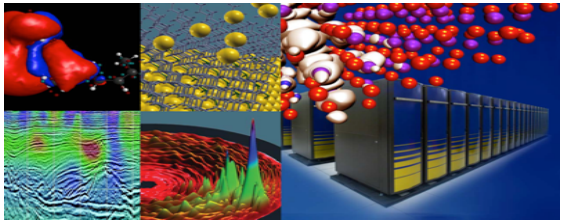
Largest funder of physical science research in U.S.



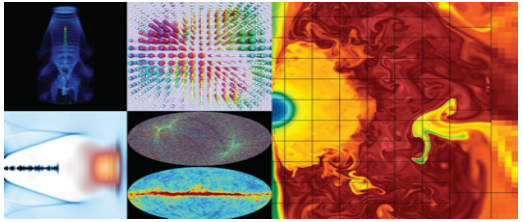
Bio Energy, Environment



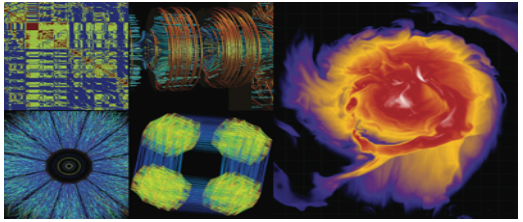
Computing



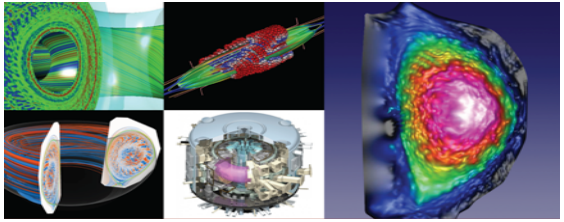
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



Nuclear Physics



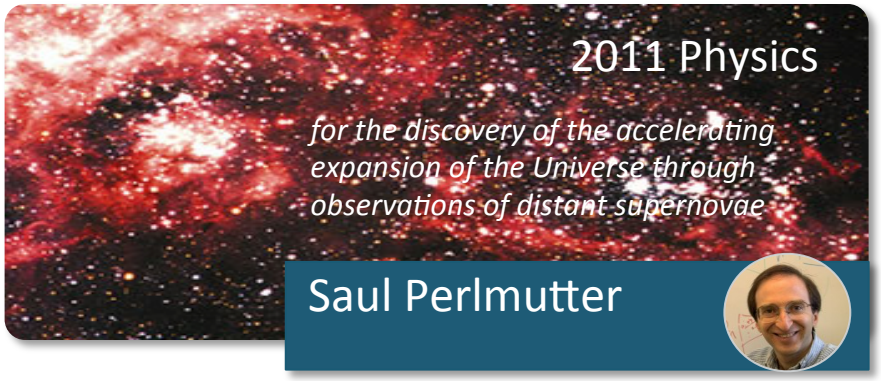
Fusion Energy, Plasma Physics

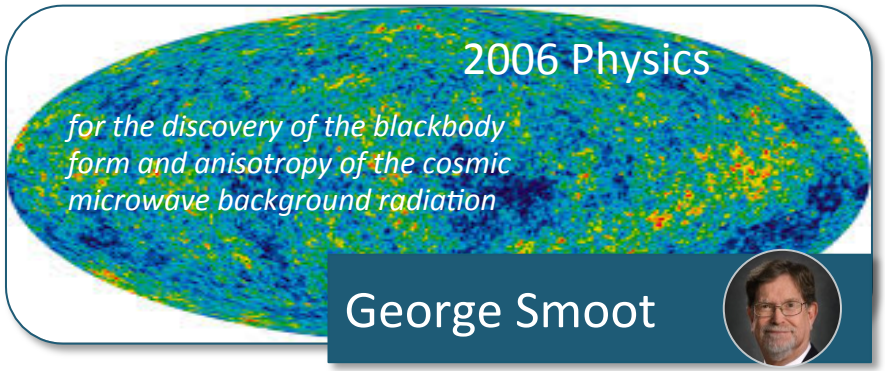
6,000 users, 48 states, 40 countries, universities & national labs

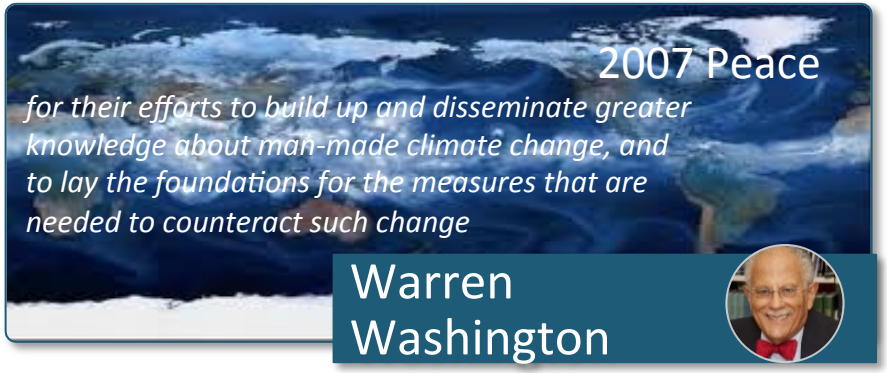
NERSC: Science First

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

Nobel-Prize Winning Users







Nobel Prize in Physics 2015

Scientific Achievement

The discovery that neutrinos have mass and oscillate between different types

Significance and Impact

The discrepancy between predicted and observed solar neutrinos was a mystery for decades. This discovery overturned the Standard Model interpretation of neutrinos as massless particles and resolved the "solar neutrino problem"

Research Details

The Sundbury Neutrino Observatory (SNO) detected all three types (flavors) of neutrinos and showed that when all three were considered, the total flux was in line with predictions. This, together with results from the Super Kamiokande experiment, was proof that neutrinos were oscillating between flavors and therefore had mass


A SNO construction photo shows the spherical vessel that would later be filled with water.

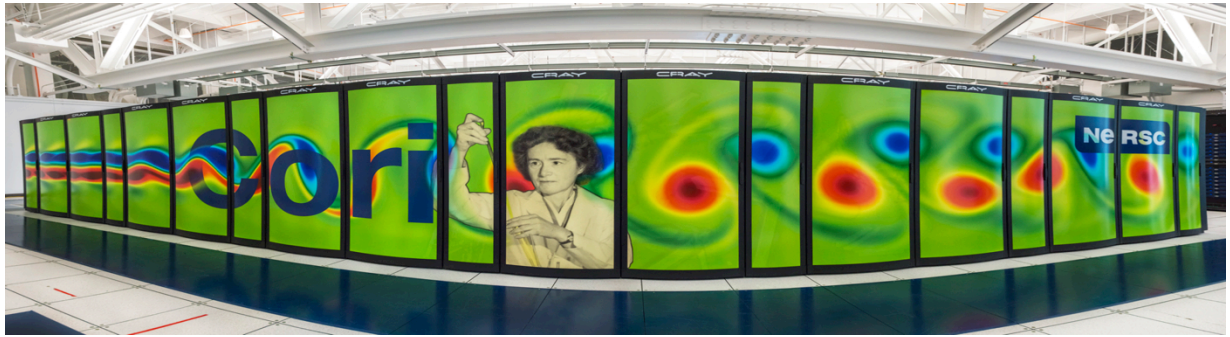
Calculations performed on PDSF & data stored on HPSS played a significant role in the SNO analysis. The SNO team presented an autographed copy of the seminal *Physical Review Letters* article to NERSC staff.

Q. R. Ahmad et al. (SNO Collaboration). Phys. Rev. Lett. 87, 071301 (2001)

Nobel Recipients: Arthur B. McDonald, Queen's University (SNO)
Takaaki Kajita, Tokyo University (Super Kamiokande)

Compute Hours

Edison
2,000 M hours



Cori Phase 1
1,000 M hours

Phase 2*
6,000 M hours

* Coming summer 2016

In 2015 scientists at NERSC

used

384,000 single-CPU-years

3,200,000,000

MPP hours of compute time

Homo erectus
~300,000 years ago

and currently store

80,000,000

5 million iPhones

Gbytes of data


NERSC