



BERKELEY LAB

Bringing Science Solutions to the World



U.S. DEPARTMENT OF
ENERGY

Office of Science

NERSC

NERSC

National Energy Research
Scientific Computing Center

Richard Gerber
NERSC Senior Science Advisor
High Performance Department Head



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U.S. DEPARTMENT OF
ENERGY

Office of Science

Office Floors and
Main Entrance

Computer Room

Shyh Wang Hall
Building 59

Mechanical Area

Today's Tour



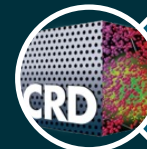
The mission of the National Energy Research Scientific Computing Center (NERSC) is to accelerate scientific discovery at the DOE Office of Science through high performance computing and data analysis.



ESnet's Mission is to enable and accelerate scientific discovery by delivering unparalleled network infrastructure, capabilities, and tools.



Wang Hall Residents



Computational
Research Divisions

Applied Math &
Computational Rsch
Scientific Data



ESnet



NERSC

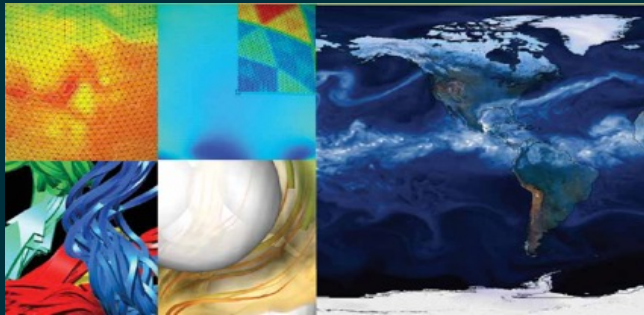
NERSC & ESnet: Mission High Performance Computing, Data, & Networking For the DOE Office of Science



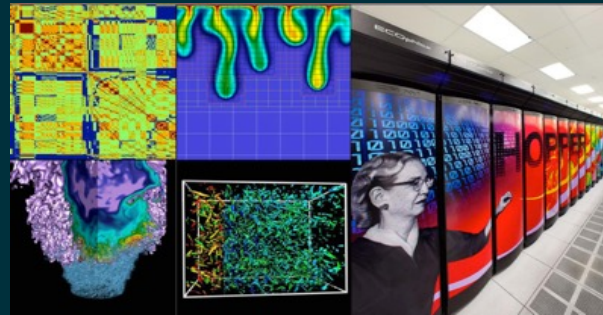
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ENERGY

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Science

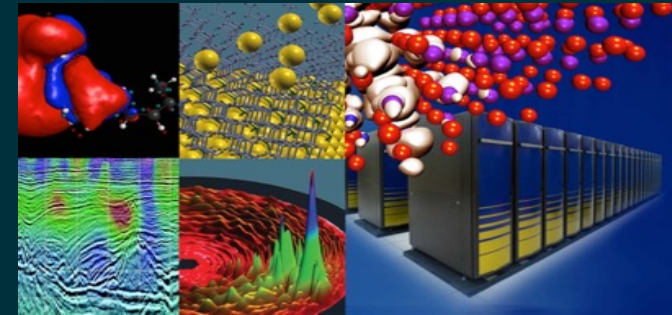
Largest funder of physical science research in the U.S.
Unclassified fundamental science and engineering



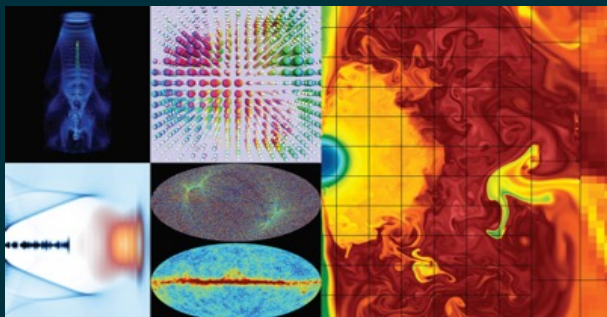
Bio Energy, Environment



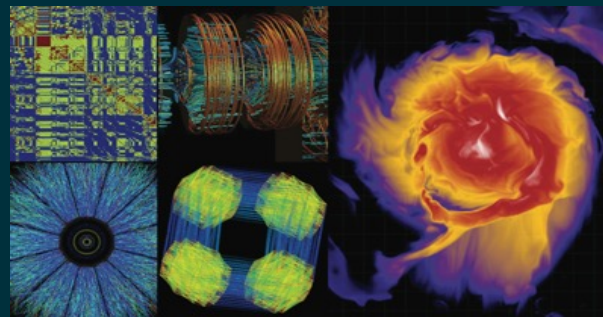
Advanced Computing



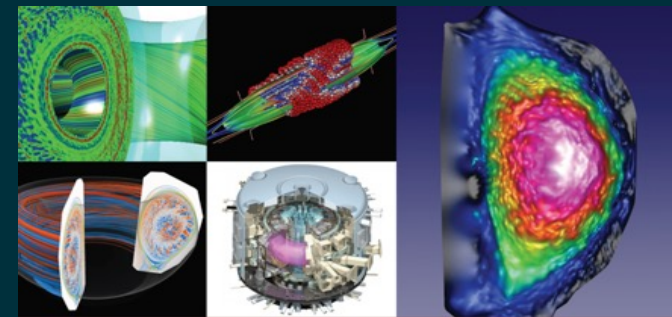
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



Nuclear Physics



Fusion Energy, Plasma Physics

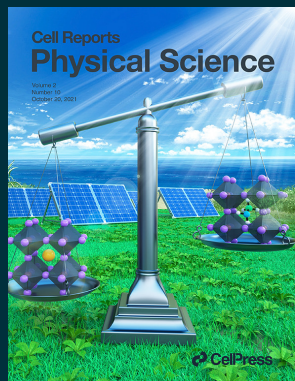
NERSC's Users Produce Groundbreaking Science



New Materials for More Efficient Solar Cells

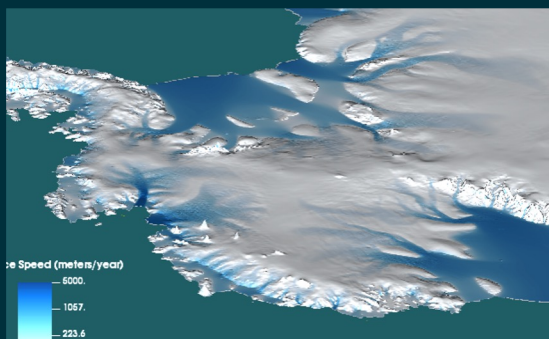
New study reveals the promise of using all-inorganic perovskite materials for solar energy conversion.

Cell Reports Physical Science



Climate & Extreme Weather

NERSC is a hub for climate and extreme weather research and the impacts on diverse communities.



Land Ice Contributions to 21st Century Sea Level Rise

Scientists quantify the effect of melting land ice on the global sea level.

Nature



World Most Advanced Coupled Earthquake-Building Simulations

Public planners can now access advanced models of different earthquake rupture scenarios will affect the public through an open-access database.

Machine Learning Technique Adds Depth, Breadth & Speed for Sky Survey Analysis

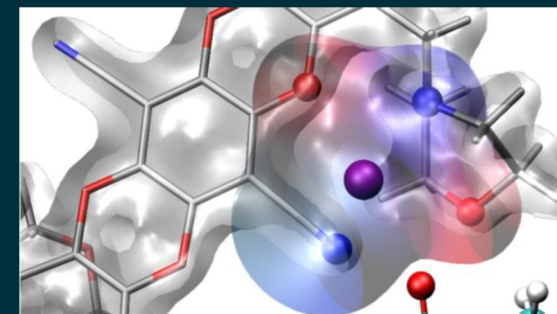
Self-supervised representation learning overcomes shortcomings of existing methods for enabling discovery.

Astrophysical Journal Letters



Breakthrough in Efficiency of Membranes for Batteries, Fuel Cells and Water Purification

Researchers have designed a membrane with "solvation cages" that can greatly speed up the flow of the desired molecules through an interface.



Nature

Perlmutter



NERSC's newest supercomputer is a Cray "Shasta" system that debuted as the 5th most powerful supercomputer in the world in 2021 (currently #8)

Designed to meet needs of large-scale simulation, data analysis, & AI/Learning

Includes both NVIDIA GPU-accelerated and AMD CPU-only nodes

35 PB All-Flash filesystem



Named after Nobel Prize Winning Berkeley Lab Scientist – and NERSC user - Saul Perlmutter

Co-discovered the accelerating expansion of the Universe ("Dark Energy")

Perlmutter: Optimized for Science



- HPE Cray System with ~4x capability of Cori
- GPU-accelerated and CPU-only nodes
- HPE Cray Slingshot high-performance network
- All-Flash filesystem
- Application readiness program (NESAP)

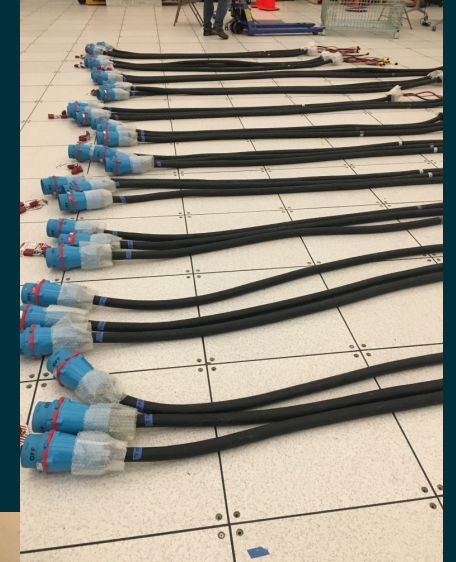
Phase 1

- 1,792 GPU-accelerated nodes
- 1 AMD “Milan” CPU + 4 NVIDIA A100 GPUs per node
- 256 GB CPU memory and 40 GB GPU high BW memory
- 35 PB FLASH scratch file system
- User access and system management nodes

Phase 2

- 3,072 CPU only nodes
- 2 AMD “Milan” CPUs per node
- 512 GB memory per node
- Upgraded high speed network: Slingshot 11
- CPU partition will match or exceed performance of the entire Cori

It's a Lot of Work to Set Up and Test a New System at this Scale



Perlmutter Phase I Arrived on February 22, 2021



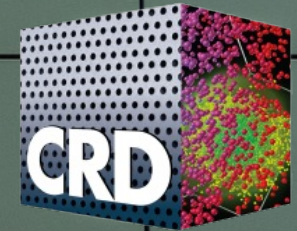
Dr. Perlmutter Started the First Science Runs

A screenshot of a terminal window titled "ssh root@login40". The terminal shows a series of ASCII art characters forming a grid-like pattern. Below this, it says "Hello, World!". Then, it says "Welcome to perlmutter! Please log current work to #shasta". The prompt "saul@perlmutter:login40:~>" is shown, followed by the command "start_all_computing". The prompt is shown again with a cursor. To the right of the terminal, there is a status table for "Perlmutter.nersc.gov". The table has columns: FEATURE, NAME, ACCOUNT, TIME, and STATE. The rows are: gpu, CatalysisDL, m3905, 0:03, RUNNING; gpu, VF3_Li, m1673, 0:03, RUNNING; gpu, NAMD_watersim, m3517, 0:04, RUNNING; gpu, BerkeleyGW, m2651, 0:04, RUNNING; and gpu, NavierStokesDL, m3885, 0:04, RUNNING. Below the table is a small video feed of a man, Saul Perlmutter, with the text "Perlmutter Accelerating Scientific Discovery through HPC" and "Saul Perlmutter" below it.

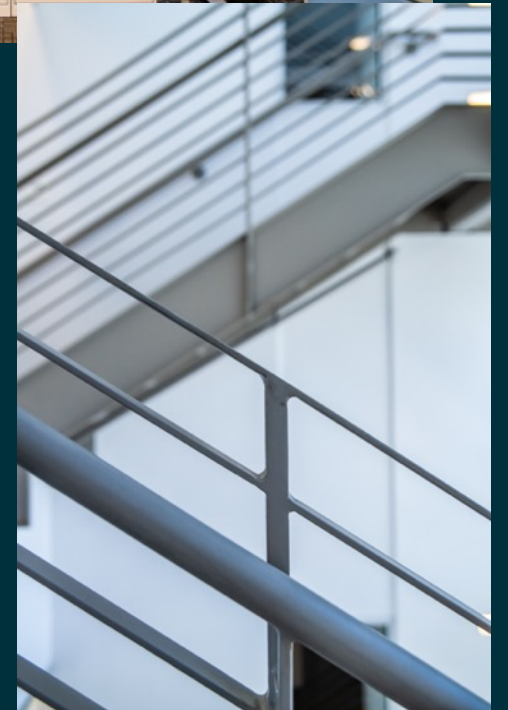
Welcome to Shyh Wang Hall



59



We Enter on the Office Floors at the Top of the Building



And Descend to the Computer Room Underneath



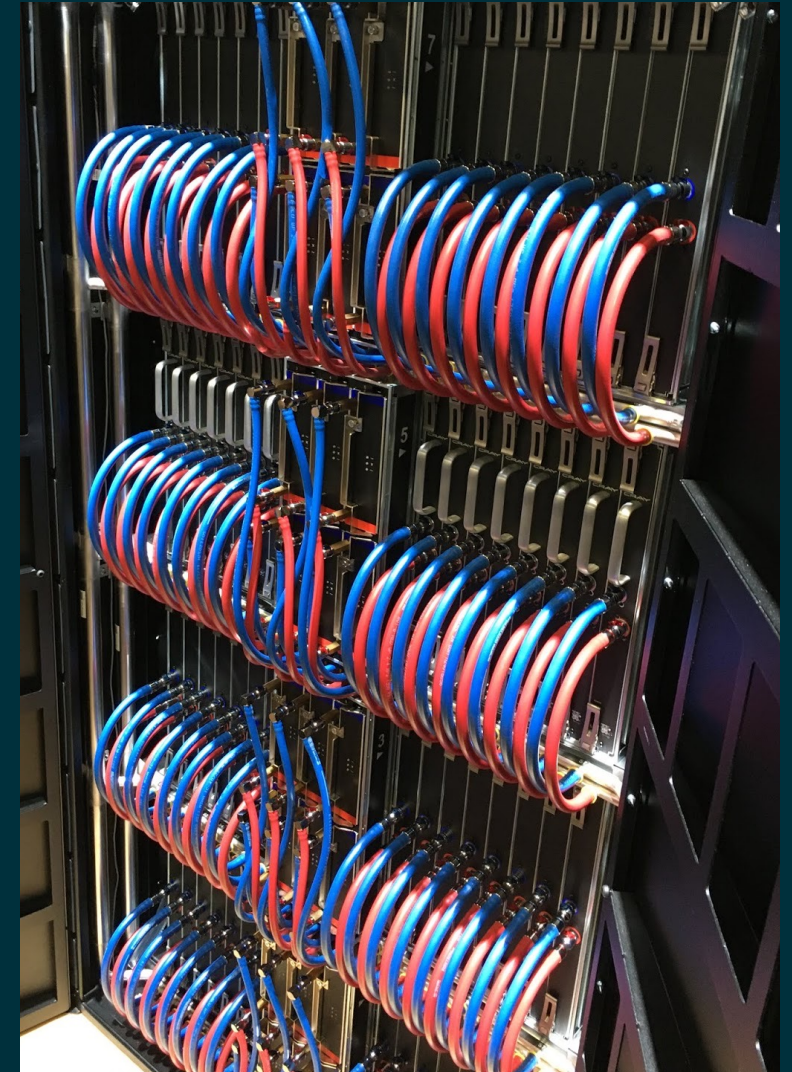
The First You'll See is the Control Room





Inside Perlmutter

CPU Compute Blade – 4 nodes (8 CPUs)



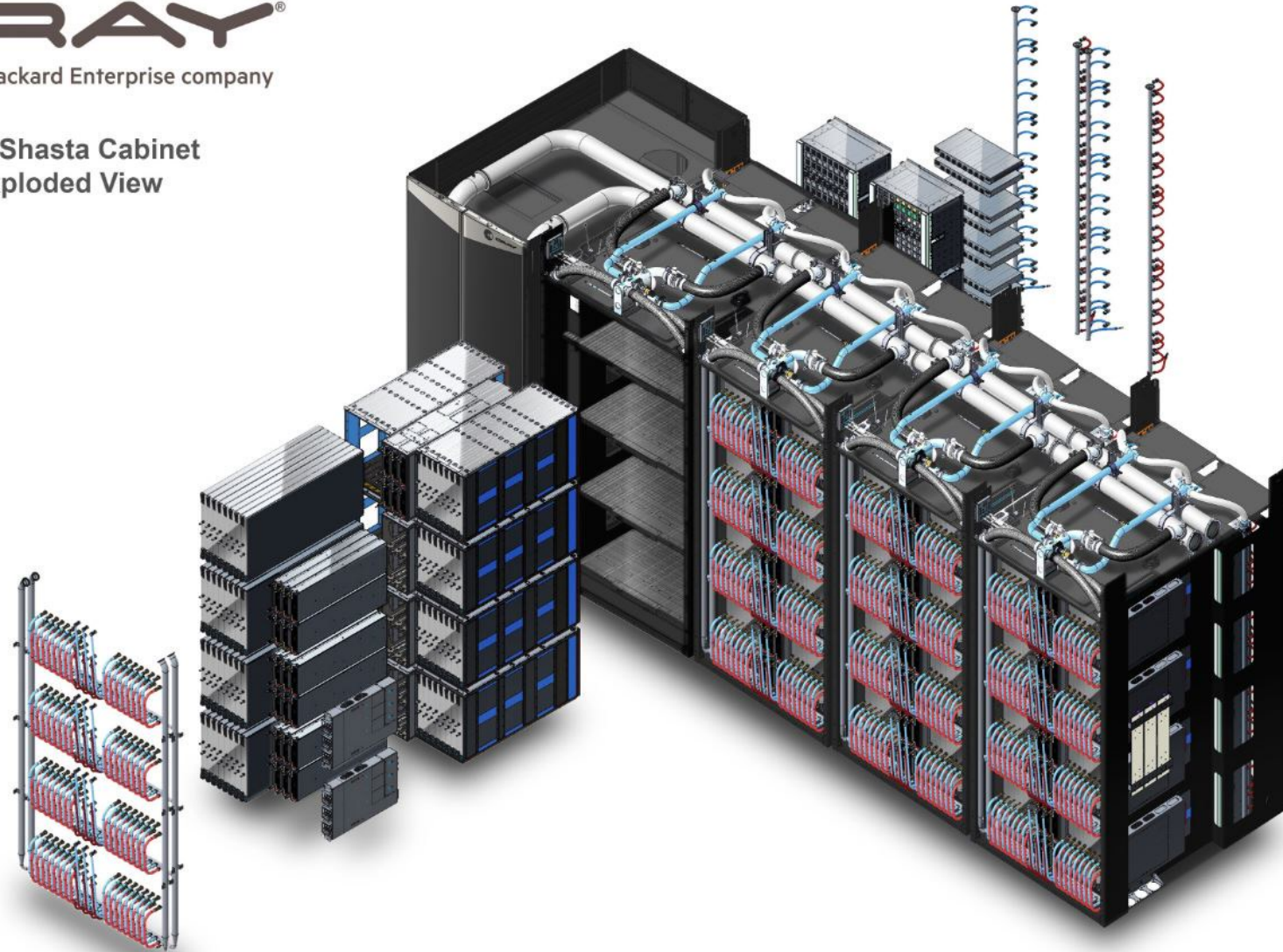
Blades in a rack with hot (red) and cold (blue) liquid cooling tubes

Perlmutter Cabinets

CRAY®

a Hewlett Packard Enterprise company

Cray Shasta Cabinet
Exploded View

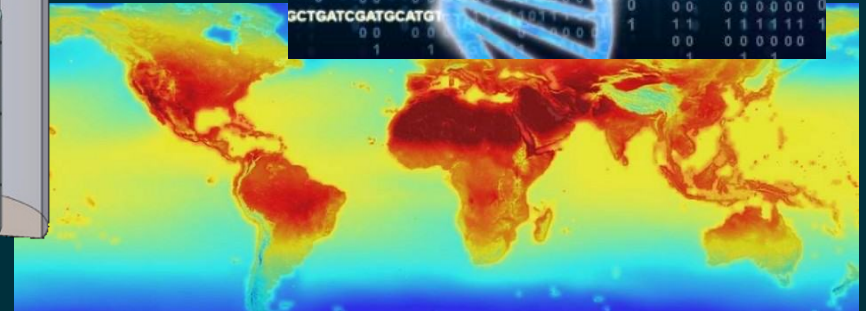
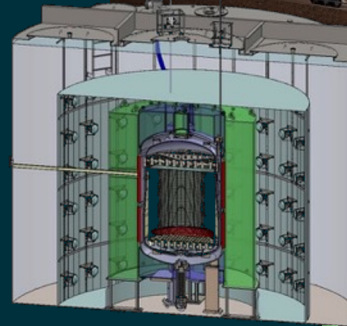
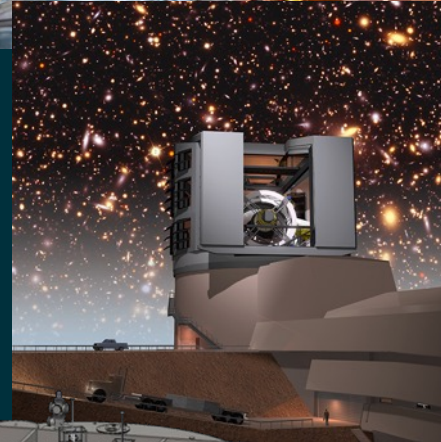
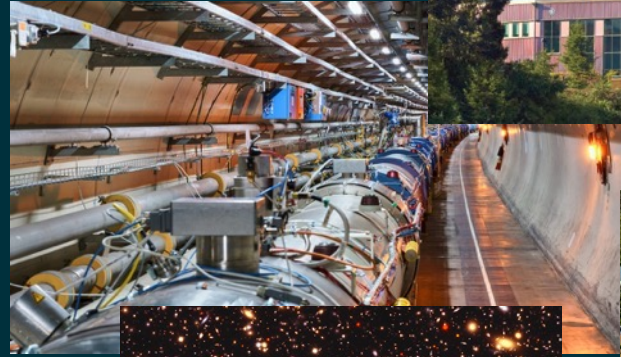


NERSC is a Big Data Center



~250 PB of
Archival
Storage

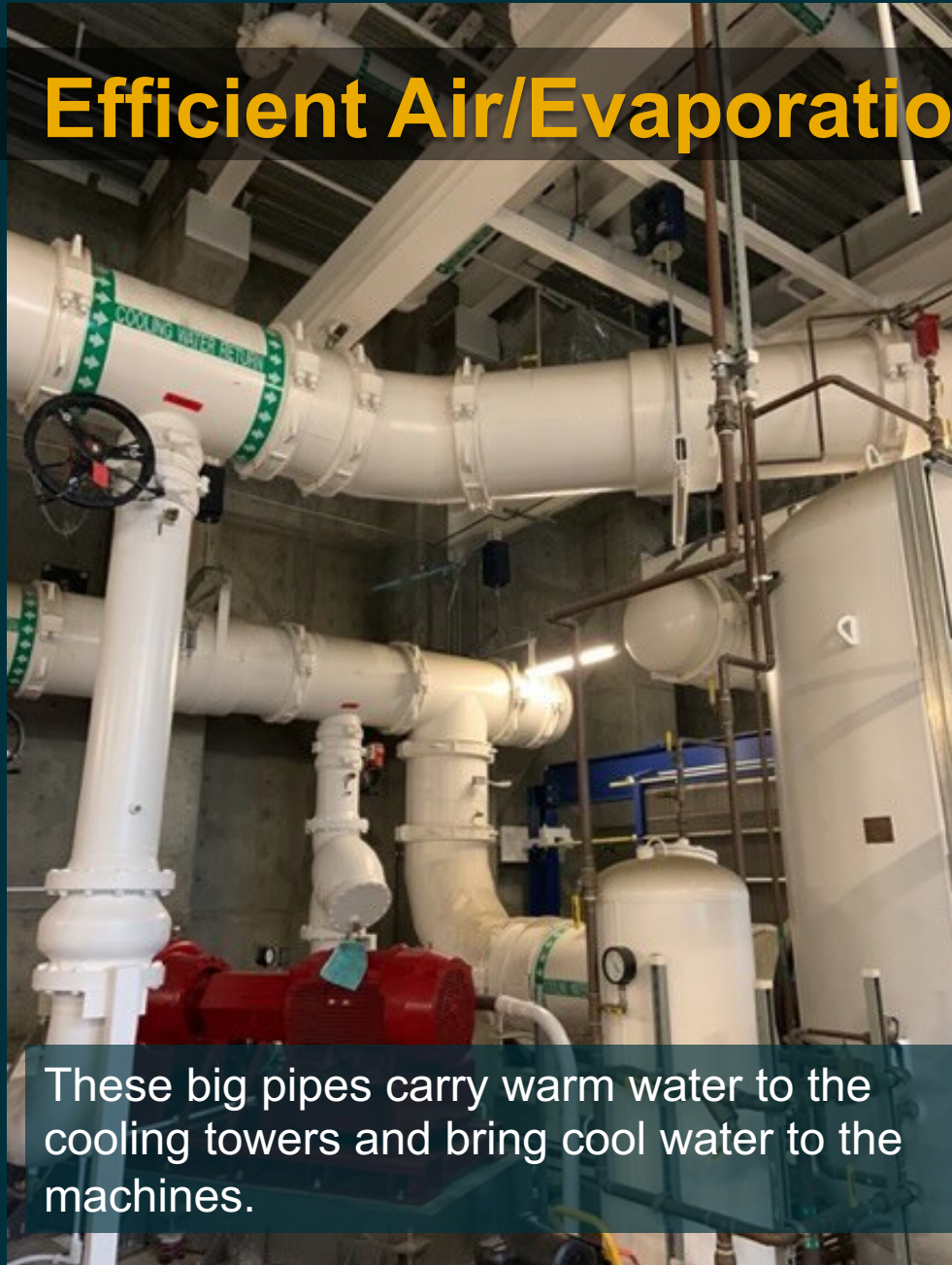
~120 PB of disk
storage in
Community File
System



Mechanical Area Below



Efficient Air/Evaporation Cooling



These big pipes carry warm water to the cooling towers and bring cool water to the machines.





Perlmutter

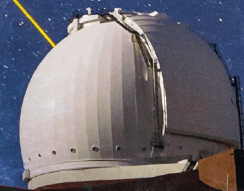
Accelerating Scientific
Discovery through HPC

Thursday, May 27
10:30am – 11:45am PT

NERSC



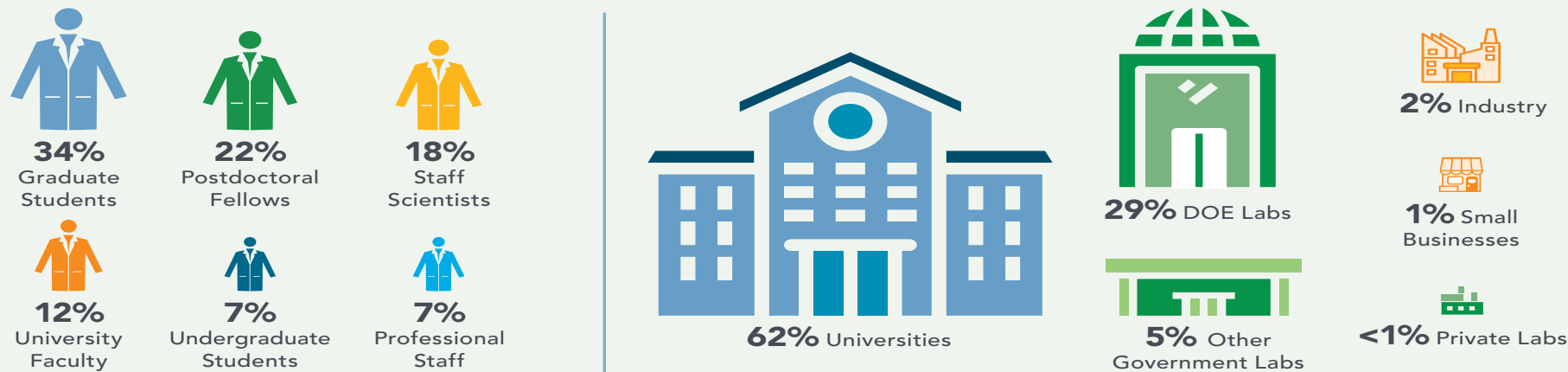
National Energy Research
Scientific Computing Center
(NERSC)



NERSC by the Numbers

NERSC BY THE NUMBERS

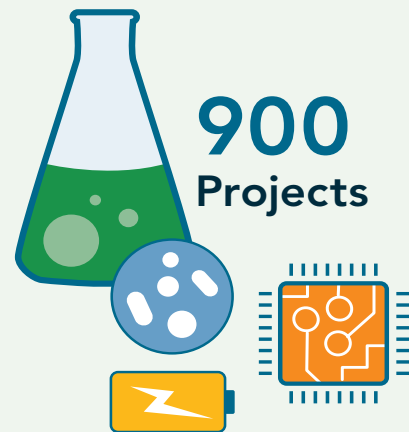
>7,000 ANNUAL USERS FROM **~1,700** Institutions + National Labs



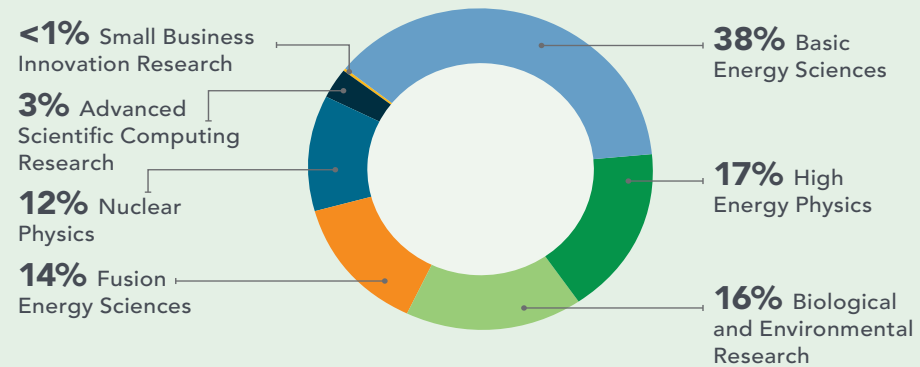
2019 NERSC USERS ACROSS US AND WORLD

50 States + Washington D.C.
46 Countries

NERSC by the Numbers



2019 DOE Office of Science Program Usage Breakdown

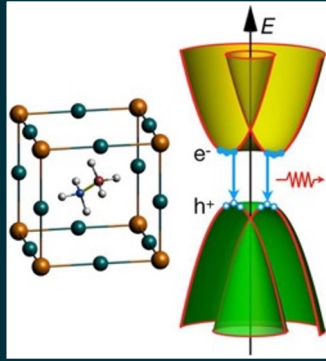


What Are NERSC Supercomputers Used For?



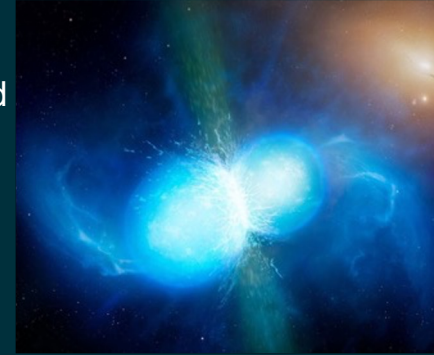
Revealing Mechanisms for Solar Cells

Researchers from UC Santa Barbara are better understanding the solar conversion efficiencies of hybrid perovskites and gaining critical insights into how they work.



Constraints on the Size of Neutron Stars

Scientists have determined with unprecedented accuracy that a neutron star with 1.4 times the mass of our Sun is packed into a sphere 11.75 km in radius.



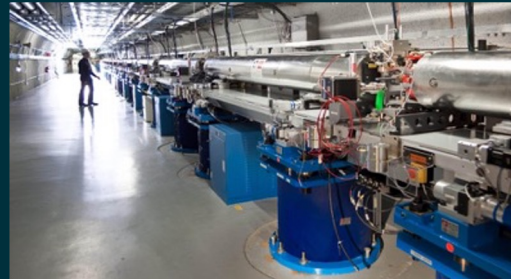
Urban Landscapes Boost Destructive Storms

A team from Pacific NW Lab found that urban landscapes and pollution can make wind gusts stronger, rain heavier, hail larger and even steer storms toward cities.



Energy Storage

Scientists from UC San Diego developed a new material that makes batteries safer, holds more charge and charges faster.



NERSC & LCLS Team Up on COVID Research

The collaboration allowed scientists to study the SARS-CoV-2 virus in unprecedented detail.

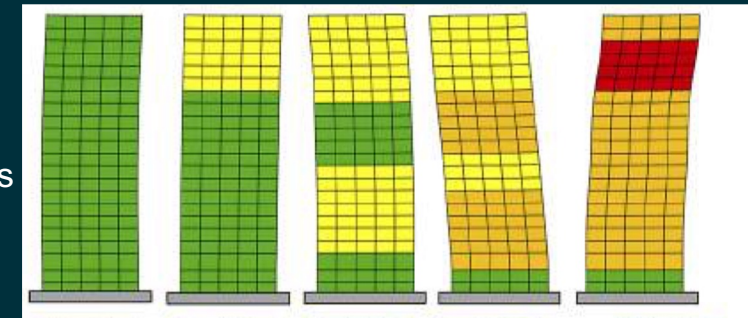
Rocket Thruster Could Propel Humans to Mars and Beyond

The proposed device can generate exhaust with velocities of hundreds of kilometers per second.



Regional Simulations of Building Response to Major Earthquakes

The study looked at many scenarios of interest to inform civic planners so they can save lives and protect infrastructure.



New Rocket Could Propel Humans to Mars and Beyond

A scientist at Princeton Plasma Physics has proposed a new type of rocket thruster that could take humankind to Mars and beyond, based on calculations performed on NERSC's Cori supercomputer.

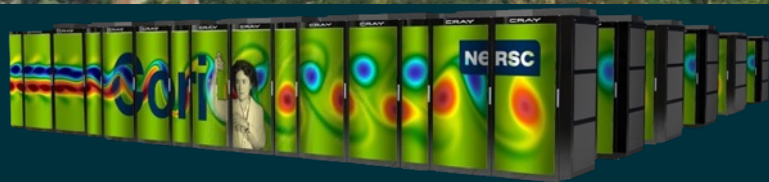
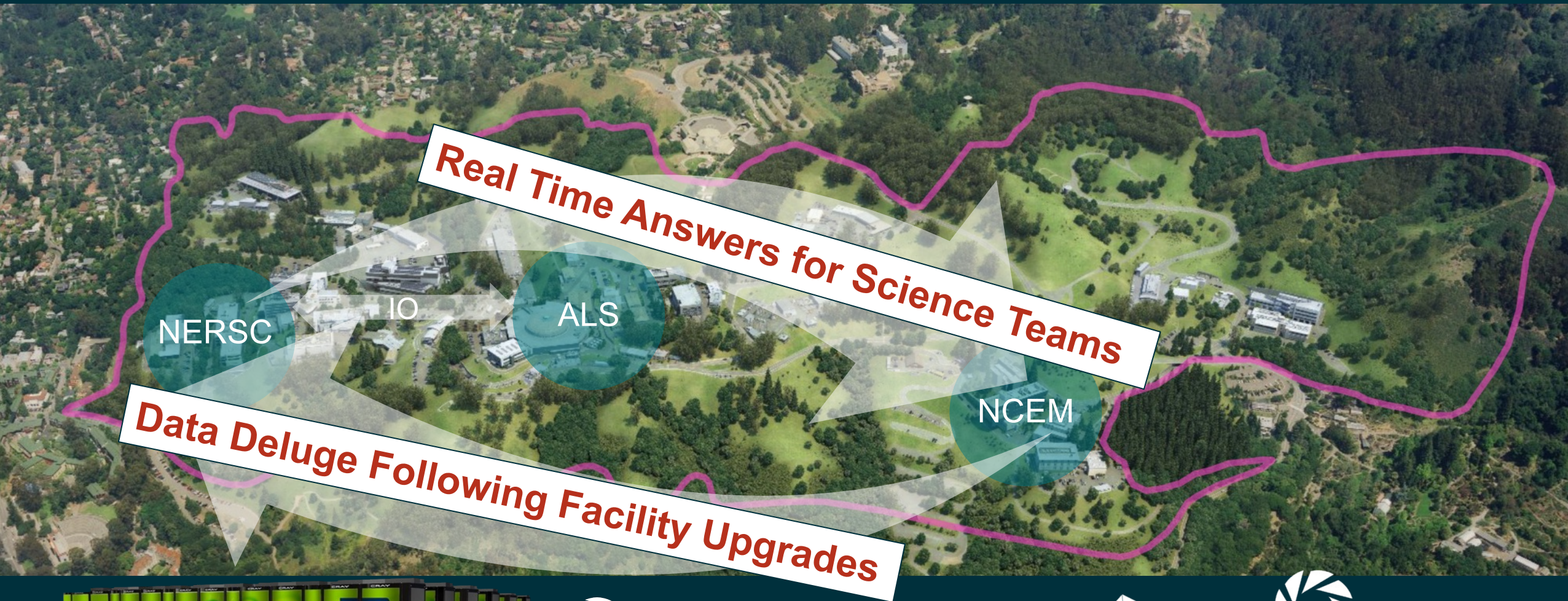
Fatima Ebrahimi showed that the new plasma thruster concept can generate exhaust with velocities of hundreds of kilometers per second, 10 times faster than those of other thrusters.

That faster velocity at the beginning of a spacecraft's journey could bring the outer planets within reach of astronauts, turning years of travel to months.



Princeton physicist Fatima Ebrahimi stands in front of an artist's conception of a rocket powered by plasma exhaust. The energetic plasma is created through magnetic reconnection, a process that occurs in the Sun and in fusion reactors.

NERSC is Teaming with Experimental Facilities





Lawrence Hall of Science

Berkeley Lab

Advanced Light Source
(ALS)

Wang Hall
NERSC
ESnet

University of
California,
Berkeley



Oakland

San Francisco

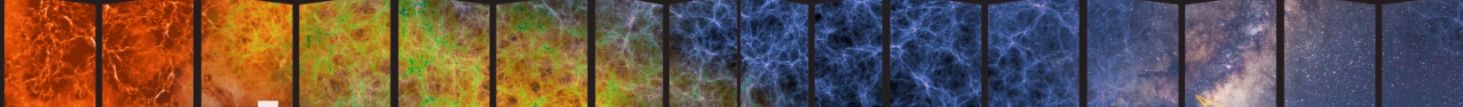
**University of
California,
Berkeley**

**Advanced Light Source
(ALS)**

**Wang Hall
NERSC
ESnet**






Berkeley Lab

First Scientific Jobs



Perlmutter

Now Computing on Perlmutter

	Catalysts for Environmentally Benign Energy Production	M Mavrikakis	U of Wisconsin - Madison
	Lattice QCD Search for Physics Beyond the Standard Model	R Gupta	Los Alamos National Laboratory
	Deep Learning for Discovery of New Catalyst Materials	Z Ulissi	Carnegie Mellon
	Simulations in Joint Center for Artificial Photosynthesis	L Wang	Berkeley Lab
	Deep Learning Assisted Simulation of Computational Fluid Dynamics	M Day	National Renewable Energy Laboratory

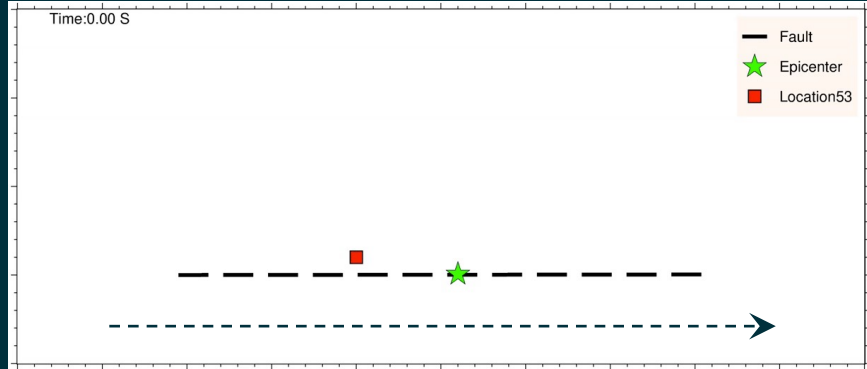
Earthquake Risk

David McCallen
University of Nevada-Reno
Berkeley Lab

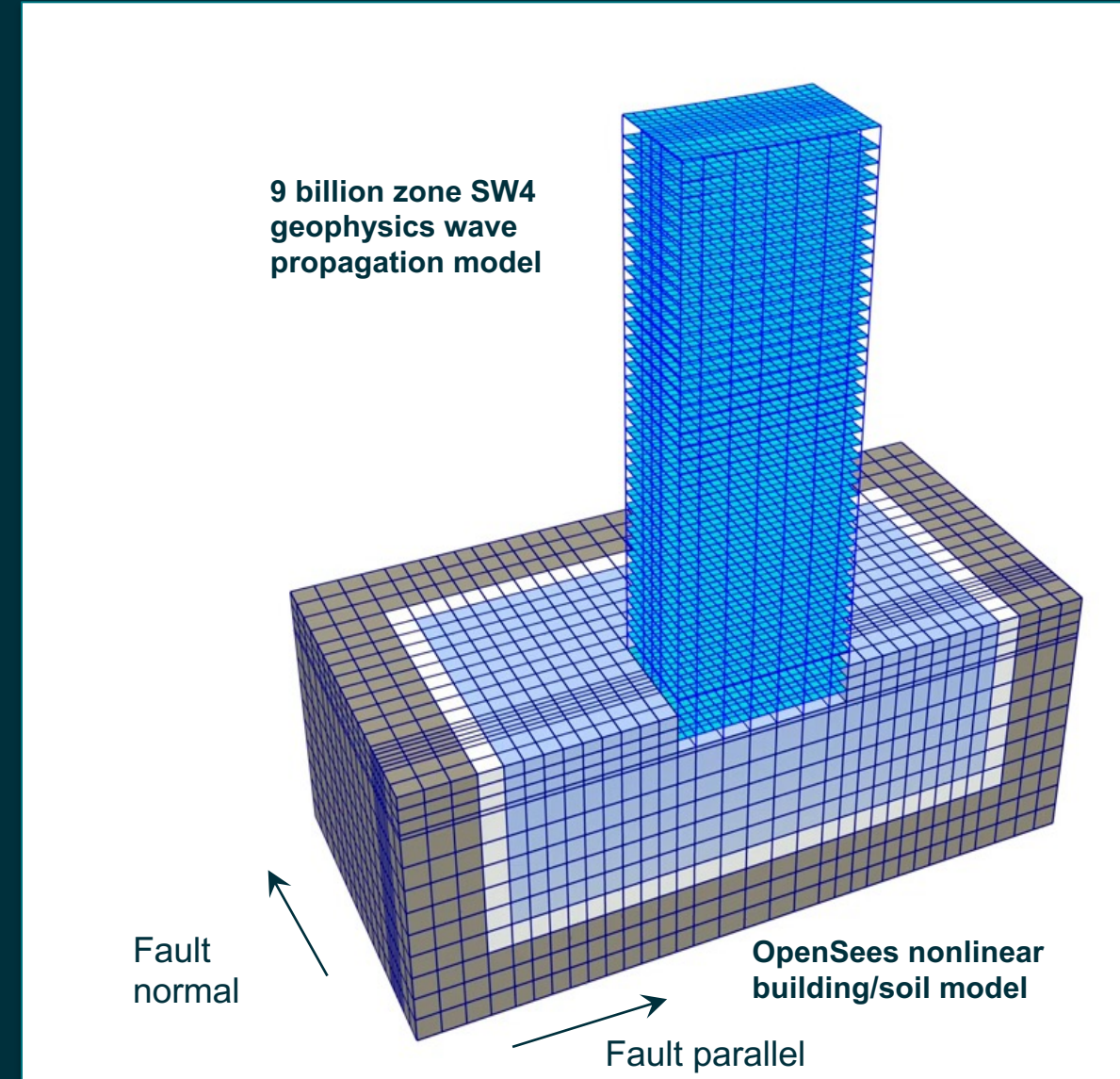
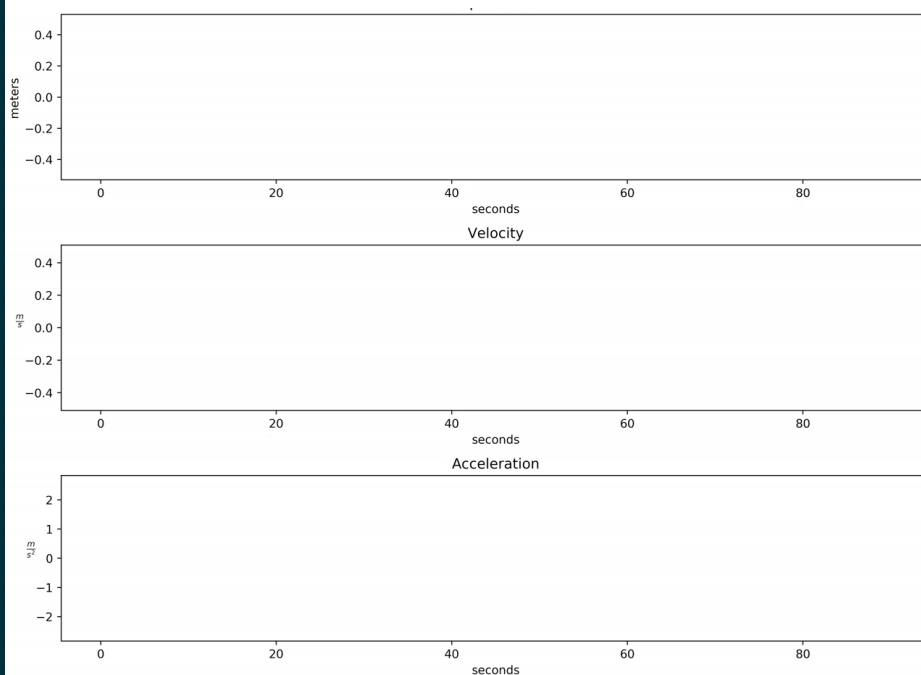
EQSIM—A multidisciplinary framework for fault-to-structure earthquake simulations on exascale computers, part II: **Regional simulations of building response**



40 story building response at location 53 (2km off the fault)



Fault parallel displacement, velocity and acceleration

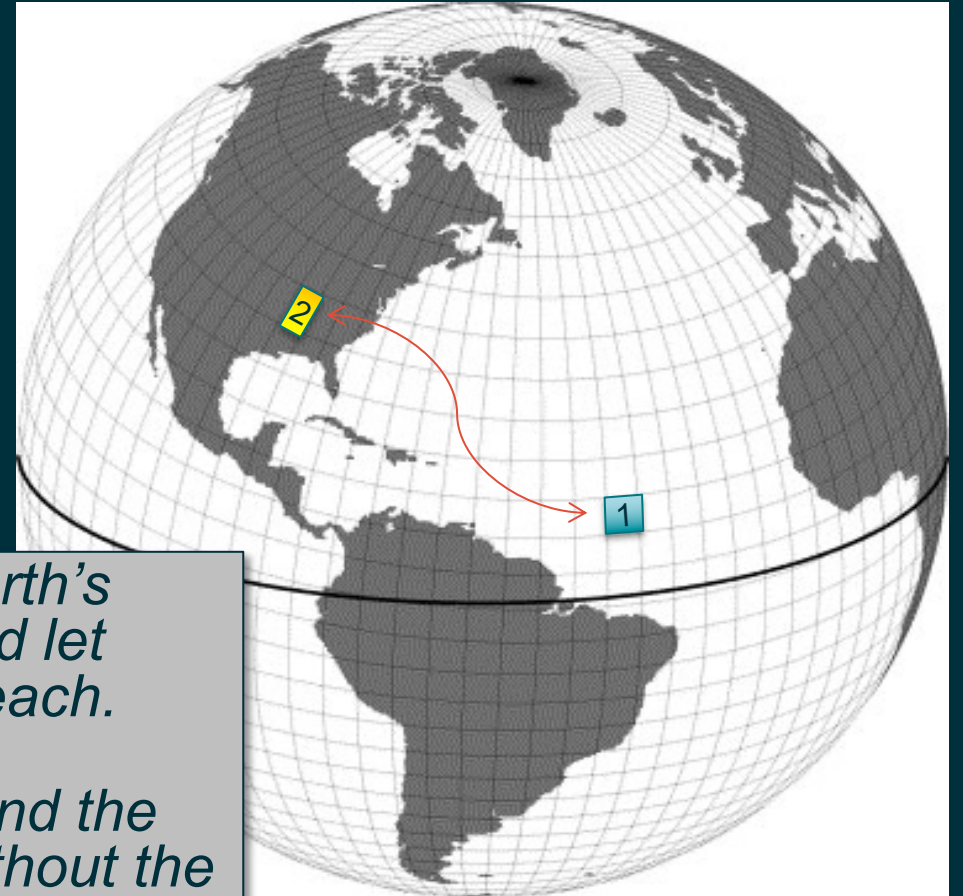


How Do All Those Processors Work Together?

- Divide a big task into smaller ones
- Each processor works on its piece
- Sends results to other processors
- Repeat until complete

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.



Processors 1 and 2 work on different parts of the problem, then send results to other processors that need the data

Let's Take a Look Around the Computer Room

