Science Solutions through Supercomputing

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Computing Sciences

Computing in Science and Engineering

Computers are used to understand things that are:

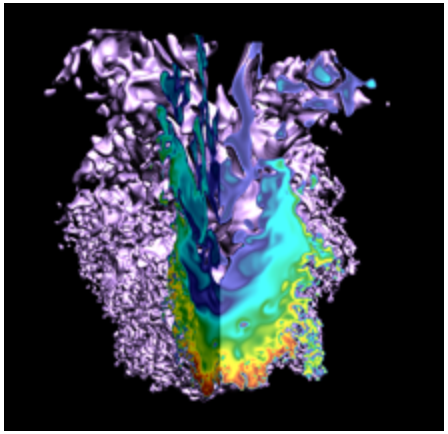
- **too big**
- **too small**
- **too fast**
- **too slow**
- **too expensive or**
- **too dangerous**

for experiments

Understanding the universe

Proteins and diseases like Alzheimer's

Industrial products and processes



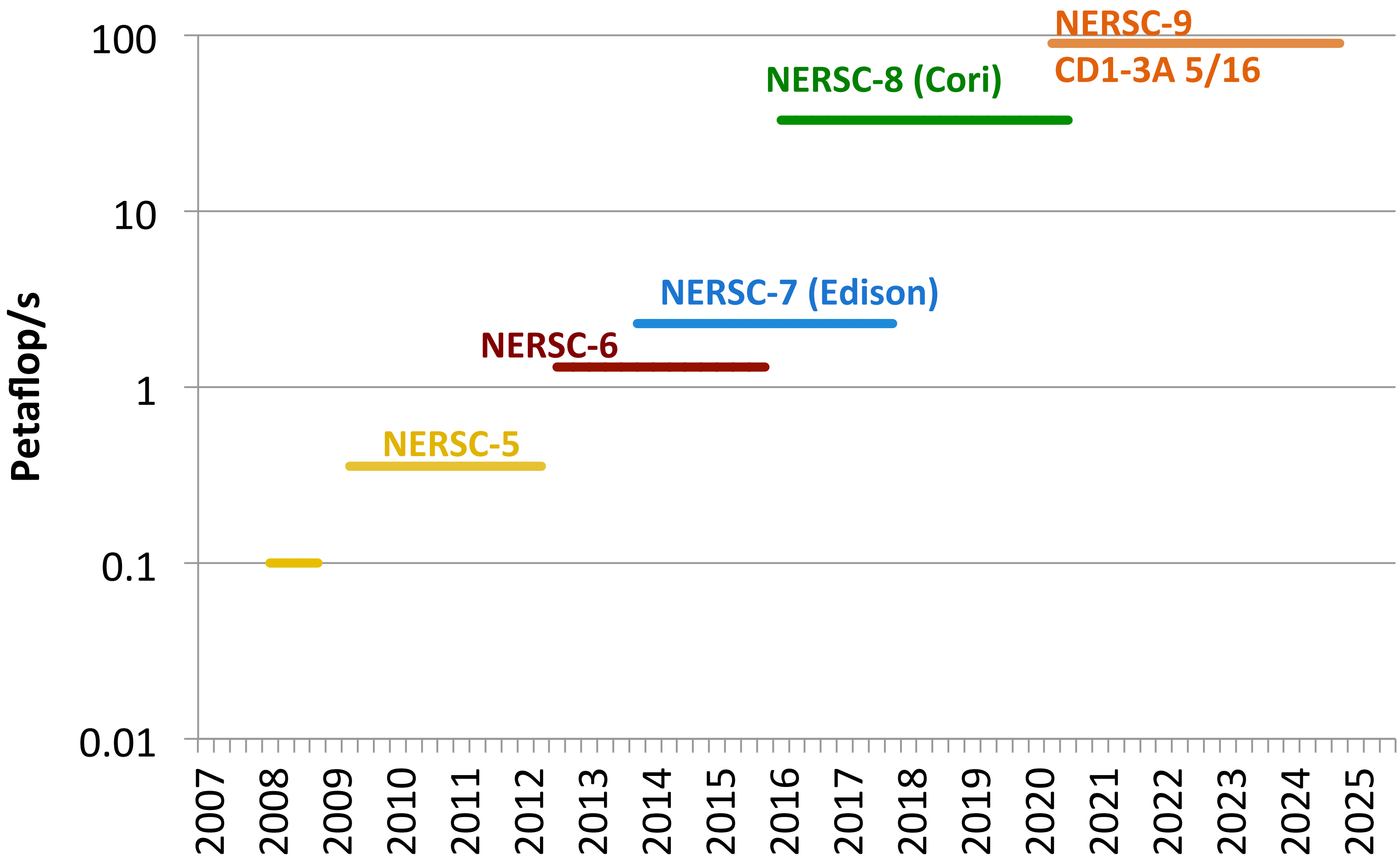
Energy-efficient combustion engines

Deploy Exascale Systems at NERSC

NERSC: the broadest, most open, widely used computing center in DOE

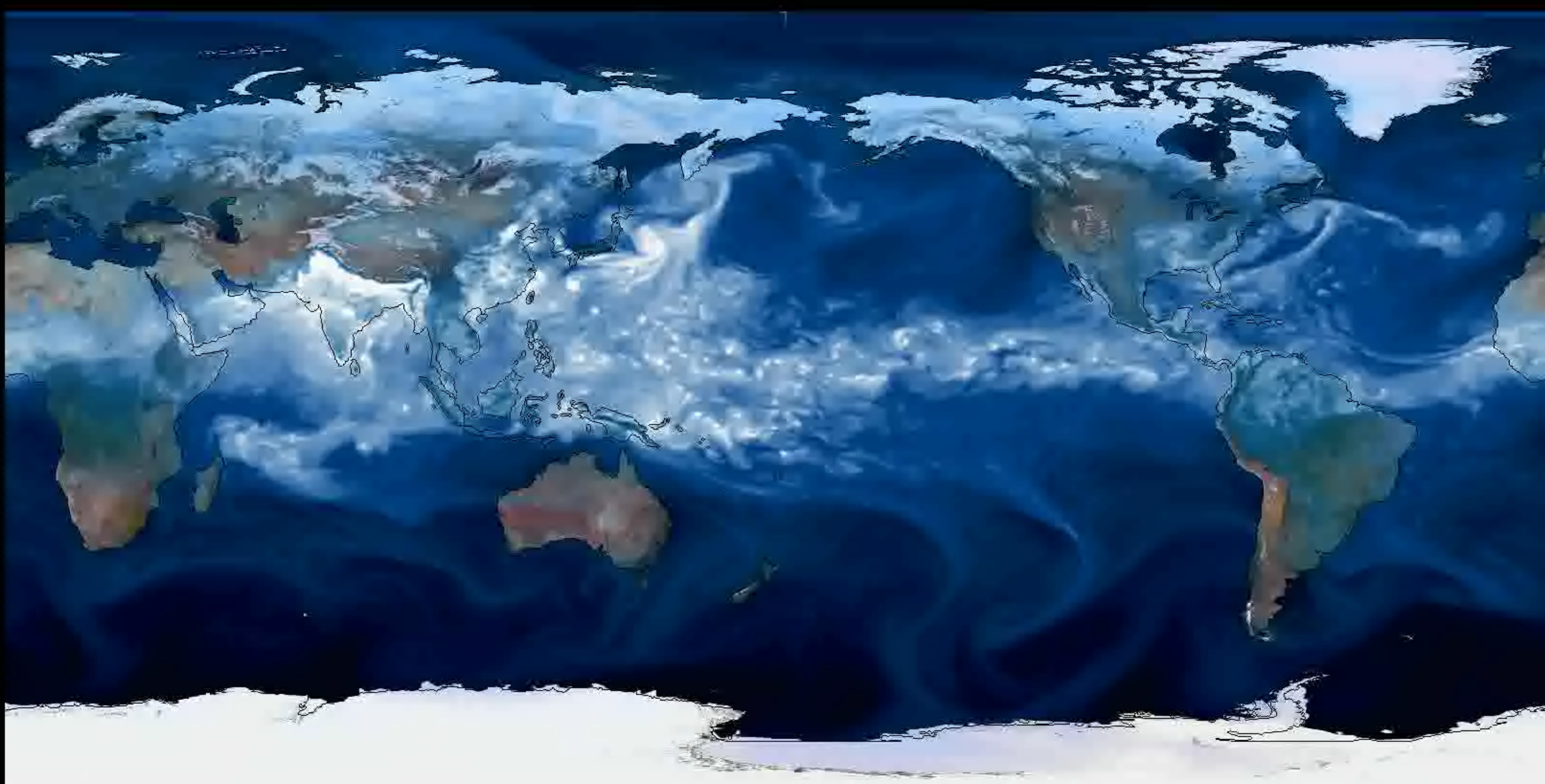
- 5000+ users, 1900+ publications, 700 codes, 5 associated Nobels
- Exascale in 2025: necessary for Office of Science mission
- Needs strong vendor ecosystem with multiple vendors/architectures

NERSC Systems Roadmap



NERSC-8 (Cori) will be the fastest computer in the US; Run at > 90% utilization

Simulations Show the Effects of Climate Changes in Hurricanes

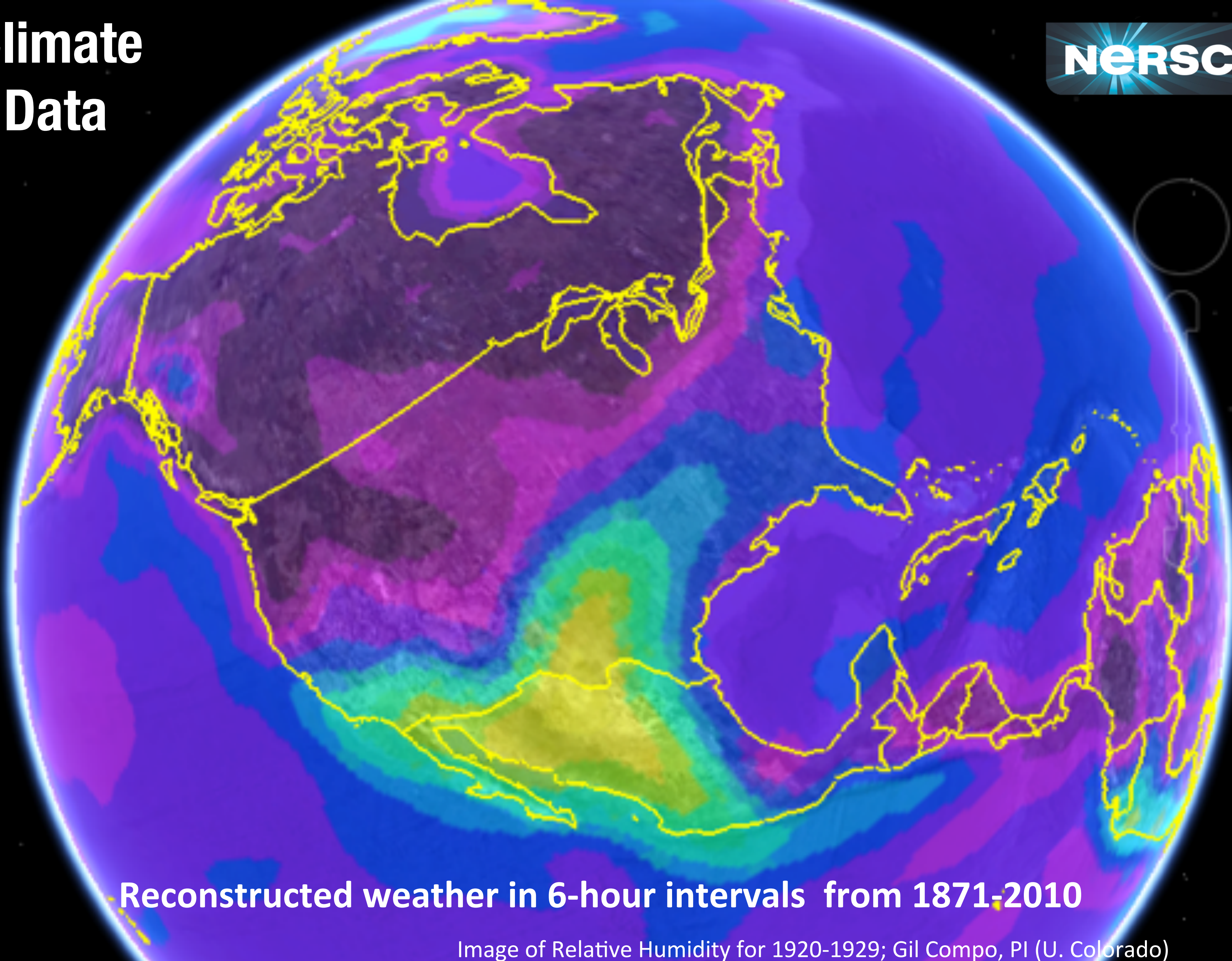


100.0
31.62
10.00
3.162
1.000

Michael Wehner and Prabhat, Berkeley Lab

August 3 1979

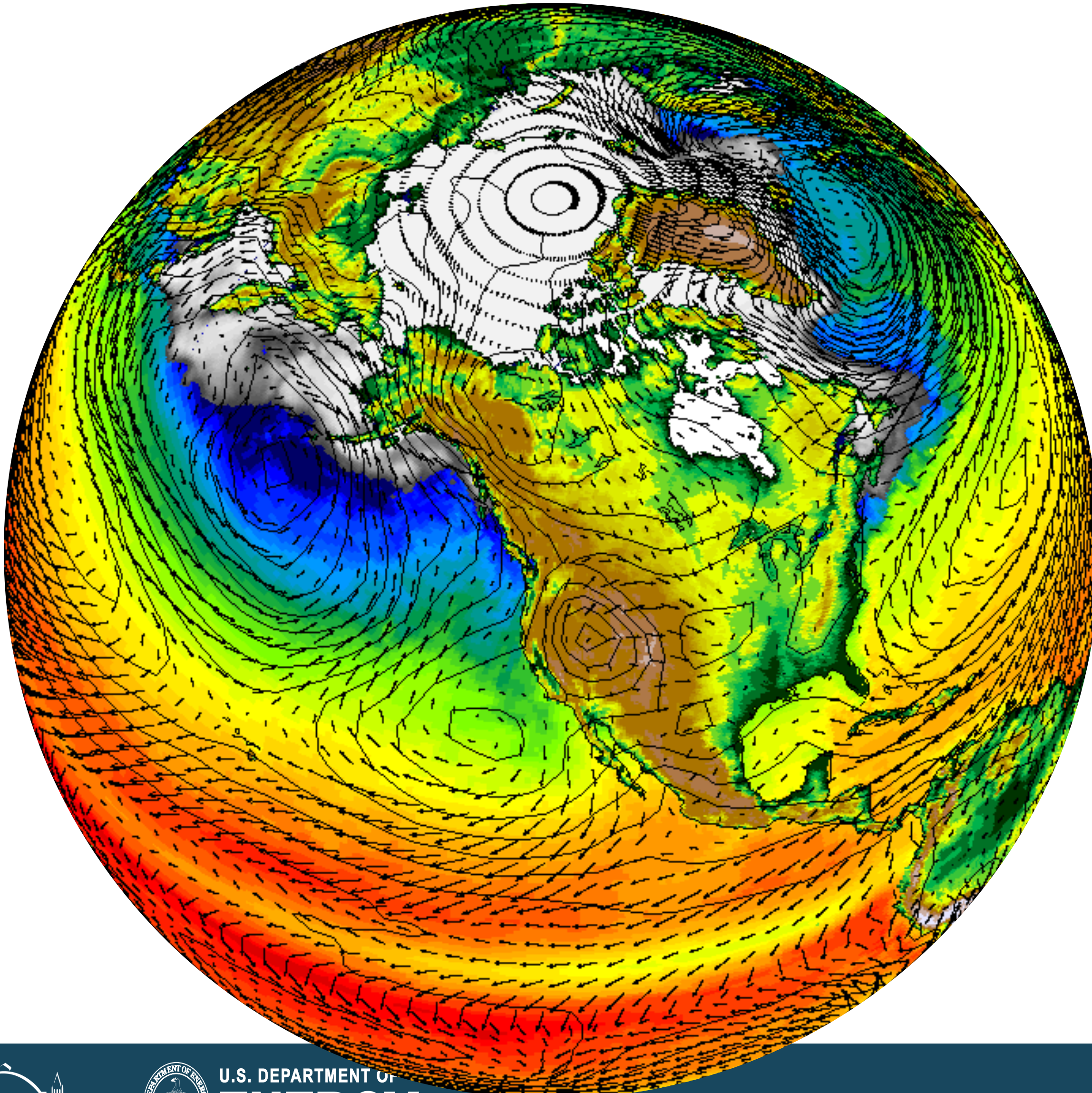
Climate Data

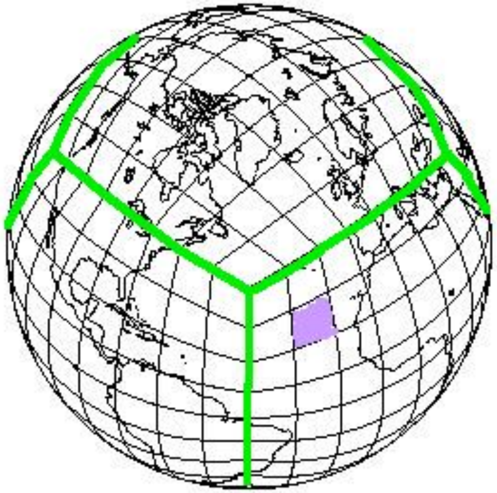


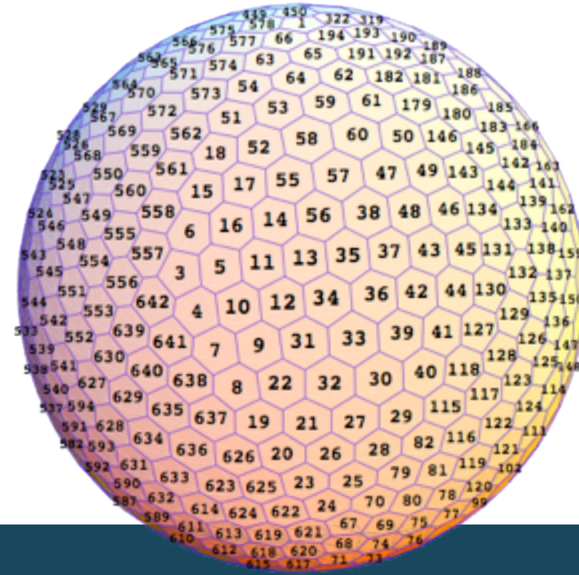
Reconstructed weather in 6-hour intervals from 1871-2010

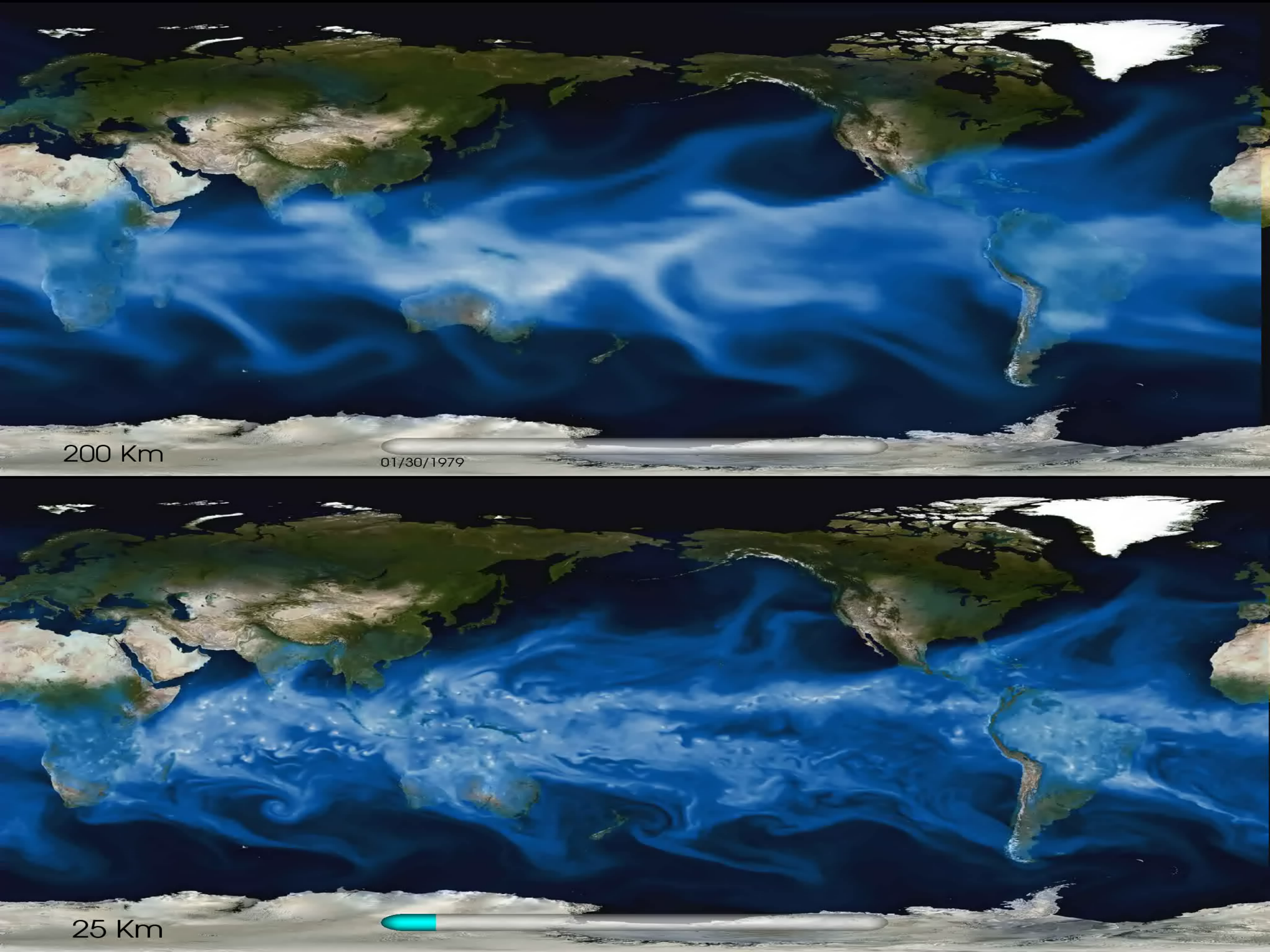
Image of Relative Humidity for 1920-1929; Gil Compo, PI (U. Colorado)

Data Structures for Simulations








200 Km
01/30/1979
25 Km

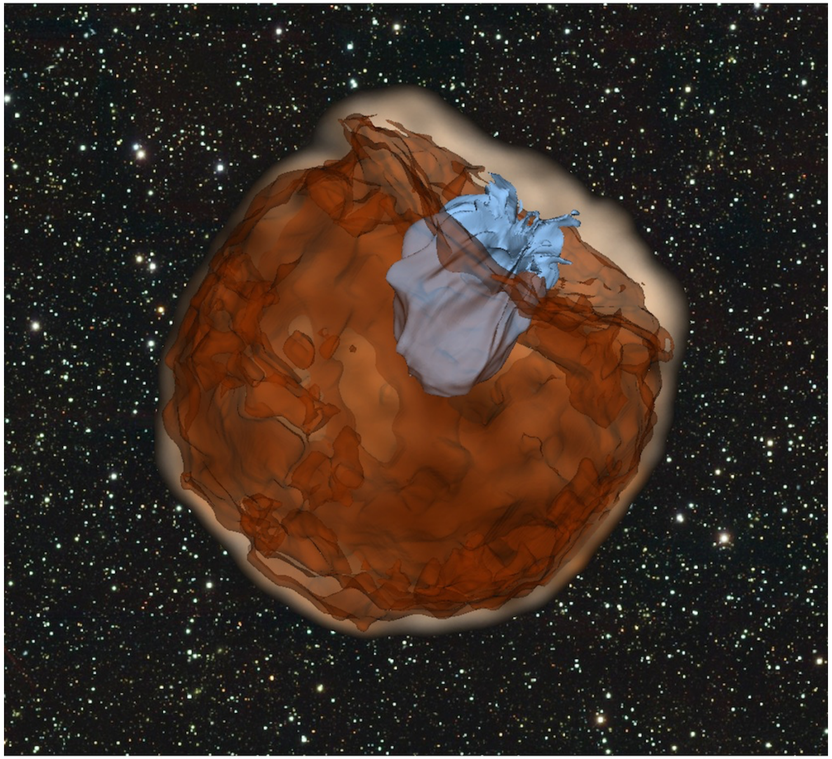
Astrophysics

Astrophysics

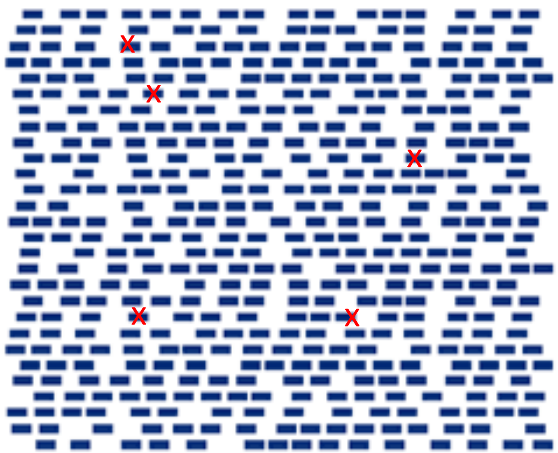
What is the source of the heaviest elements? Improve understanding of the rapid neutron capture process (the r-process).

Simulation Challenge Problems

- ✓ Fully self-consistent calculations of all of the main proposed r-process scenarios: core-collapse supernovae, neutron star mergers, and accreting black holes
- ✓ Calculation of related stellar explosions: novae, x-ray bursts and thermonuclear supernovae
- ✓ Requires advanced multi-group neutrino radiation transport

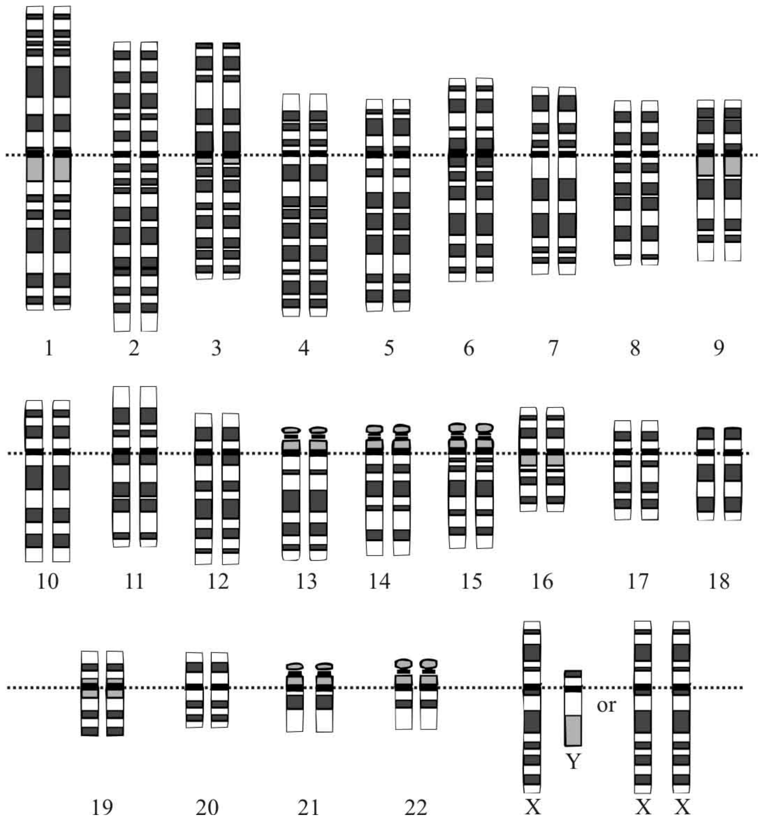


Genome Assembly



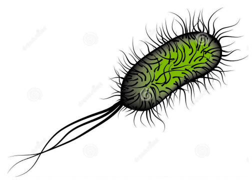
>>10^9 sequencing reads

36 bp - 1 kb



3 Gb

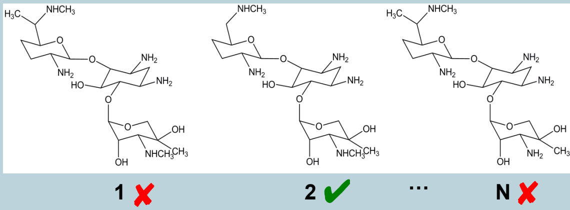
Genomes vary in size

Organism	Genome size (in billion bases)	Typical read data size
E. Coli 	0.5	3 Gb
Hagfish 	1.5	300 Gb
Human 	3	650 Gb
Wheat 	17	1200 Gb
Salamander 	20	1400 Gb

Metagenome Analysis

Biofoundry: Rapid Production of Antimicrobials

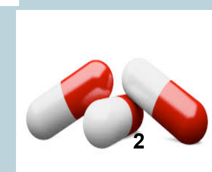
New antibiotic-resistant pathogen



Screen drug variants for efficacy

Stockpiled vials of cells to produce drug variants

Distributed fermentation drug production facilities



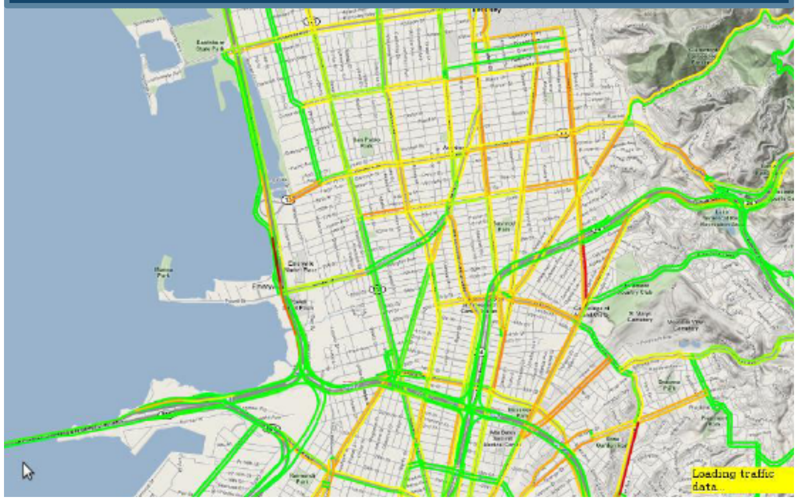
Rapid surge production of effective drug variant

Grand Challenge:

- Discover new and improved antimicrobials for human, animal, and plant pathogens
- Rapidly identify an effective antibiotic and surge its production at distributed sites

Science in embedded sensors: Internet of Things

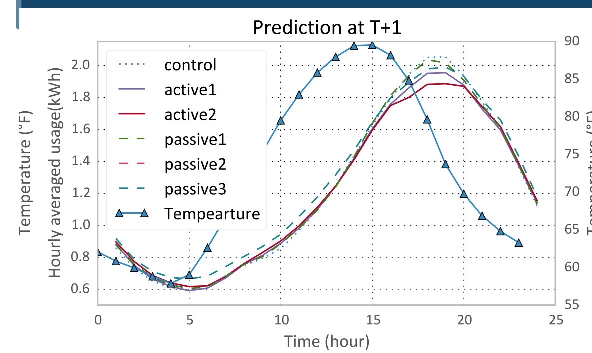
Transportation Modeling



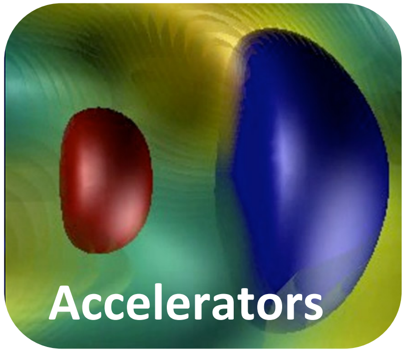
Power Grid Modeling

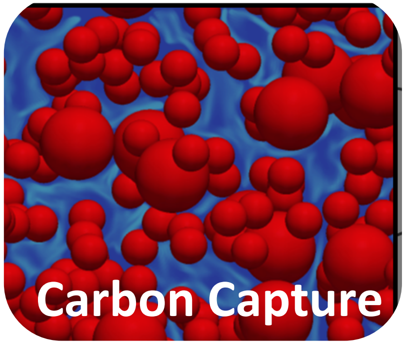
Scenario Prediction, Planning

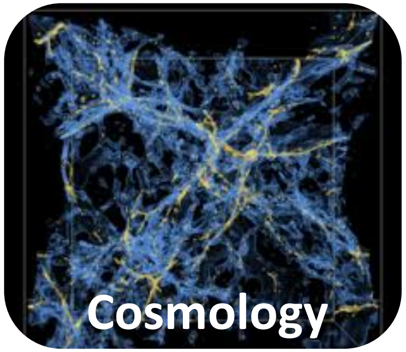
Decision Science

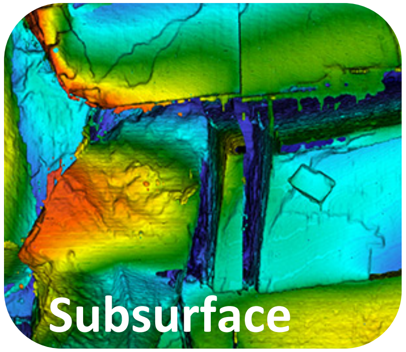


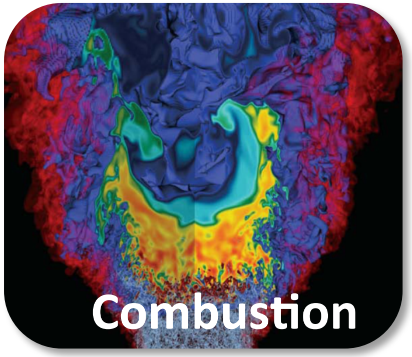
Use Math Leadership to Maximize Exascale Science

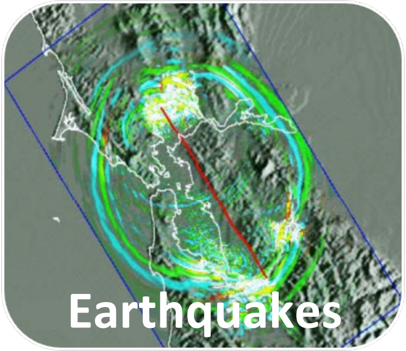


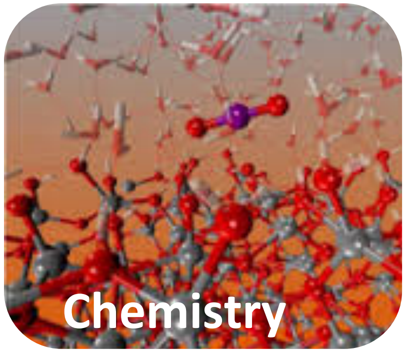


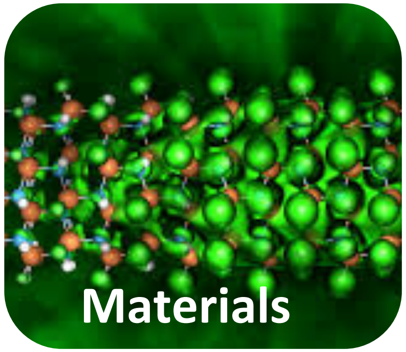


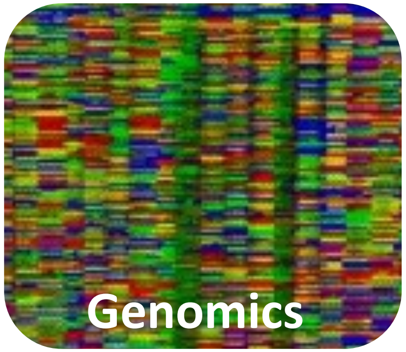


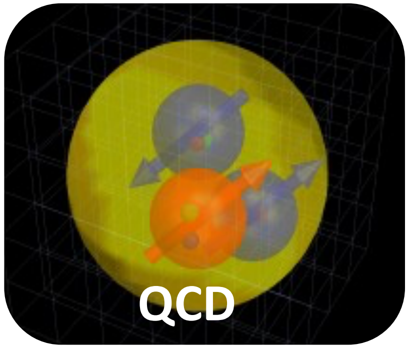












Discovery unconstrained by geography via ESnet

Transform global science networks.

OSCARS

Create information and tools for optimal network use.

SDN
Software Defined Networking

Pioneer architectures, protocols, applications.

DMZ image credit: SDSC

Changing Science through a "Superfacility"

Enabling New Scientists

17-year-old Brittany Wegner creates breast cancer detection tool that is 99% accurate on a minimally invasive, previously inaccurate test.

Machine Learning + Online Data + Cloud Computing