Computational Math and Science

How Mathematics Will Help Save The World

Juan Meza
Professor Applied Mathematics
Dean, School of Natural Sciences, UC Merced

WHICH ONE OF THESE DO **NOT** USE MATH?

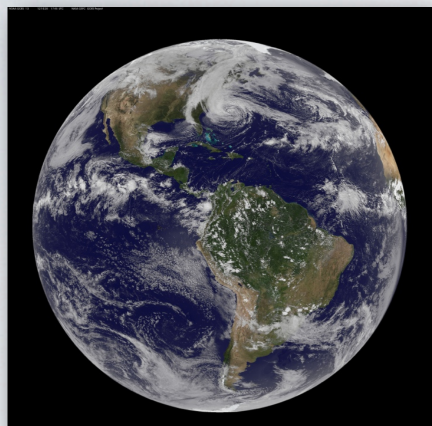
A) Finding prime numbers: 2, 3, 5, 7, 11, 13, ...

B) Predicting climate change

C) Understanding biological function

D) Building an invisibility cloak

Let's do an experiment



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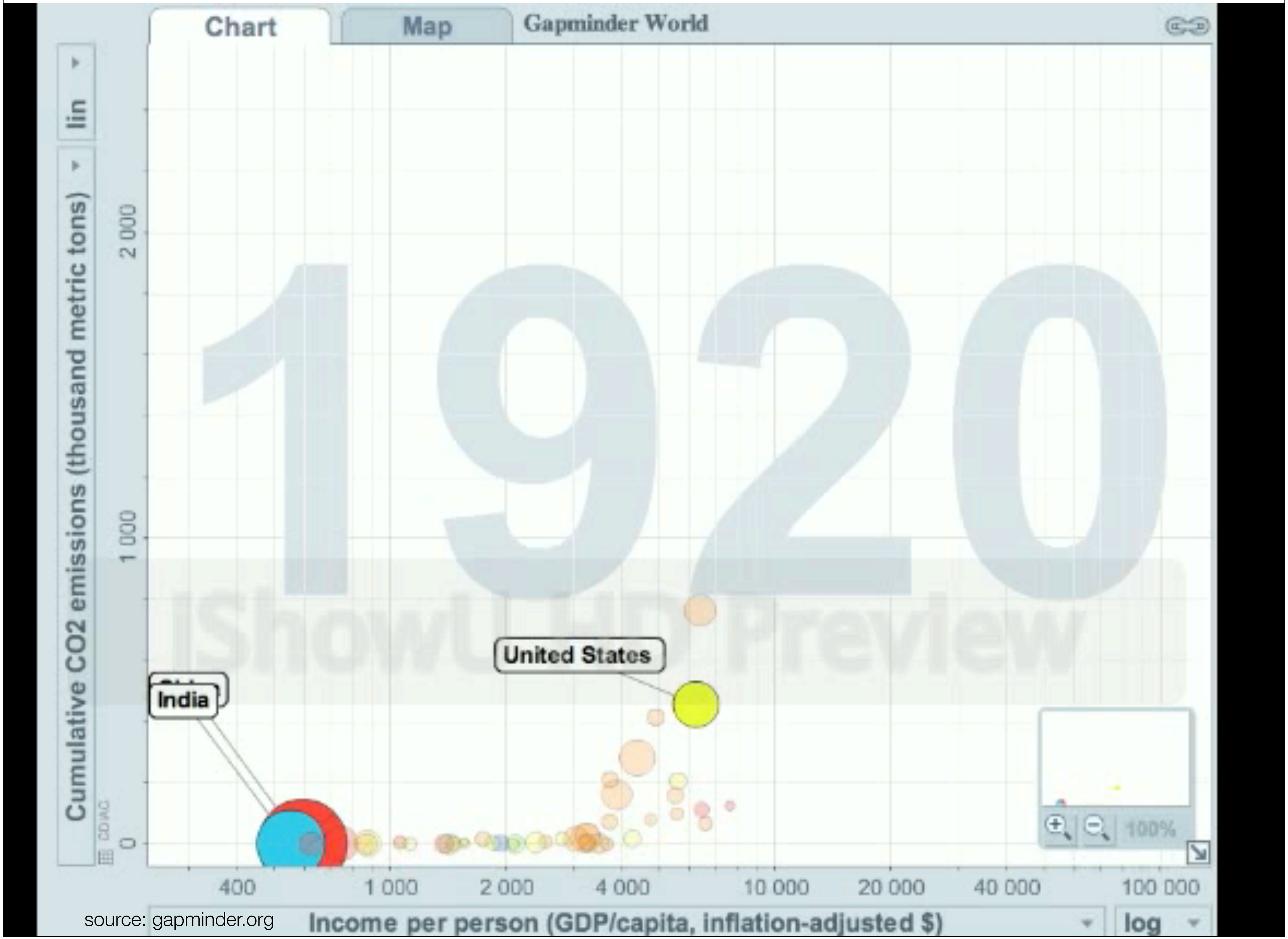
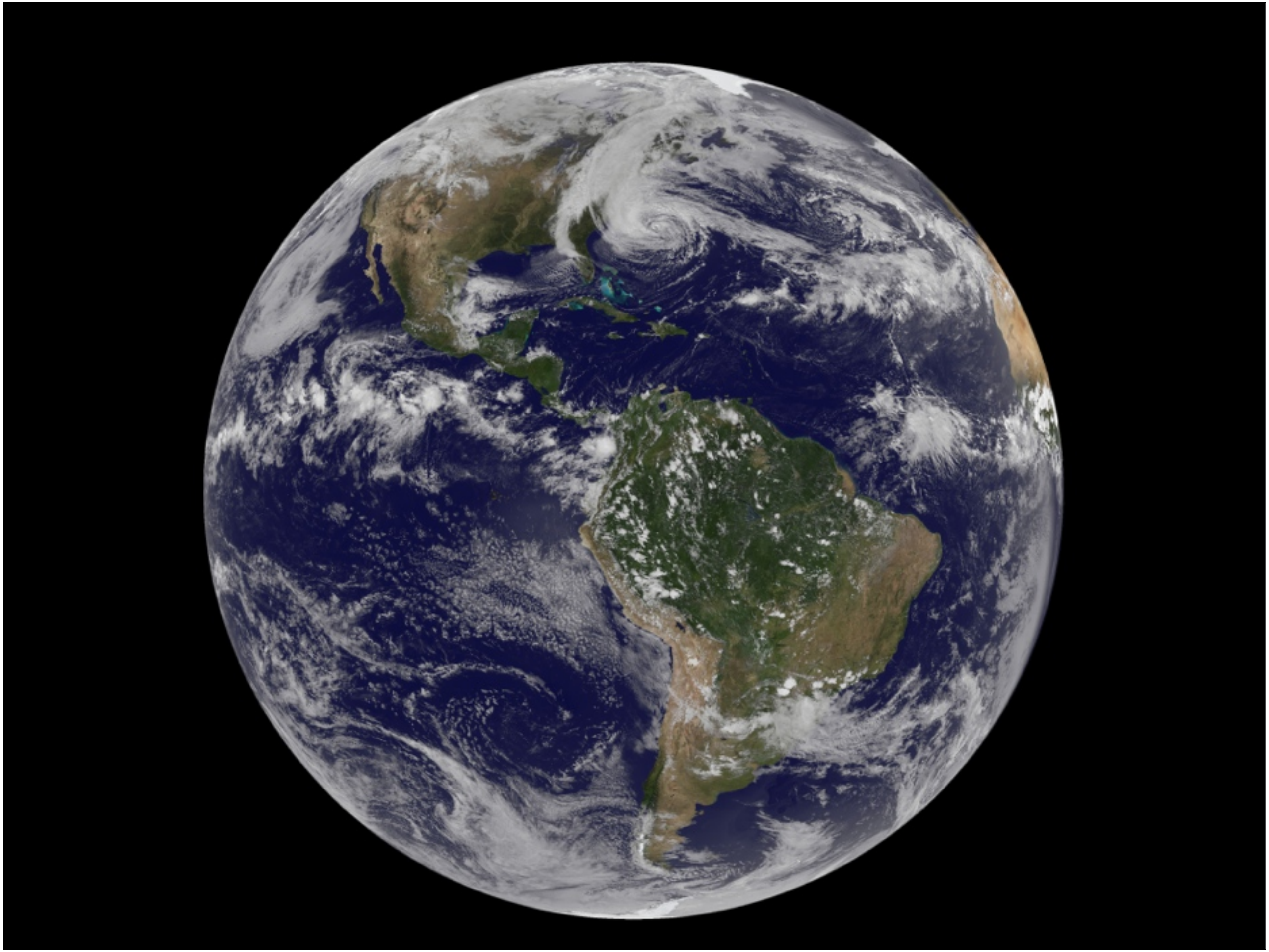
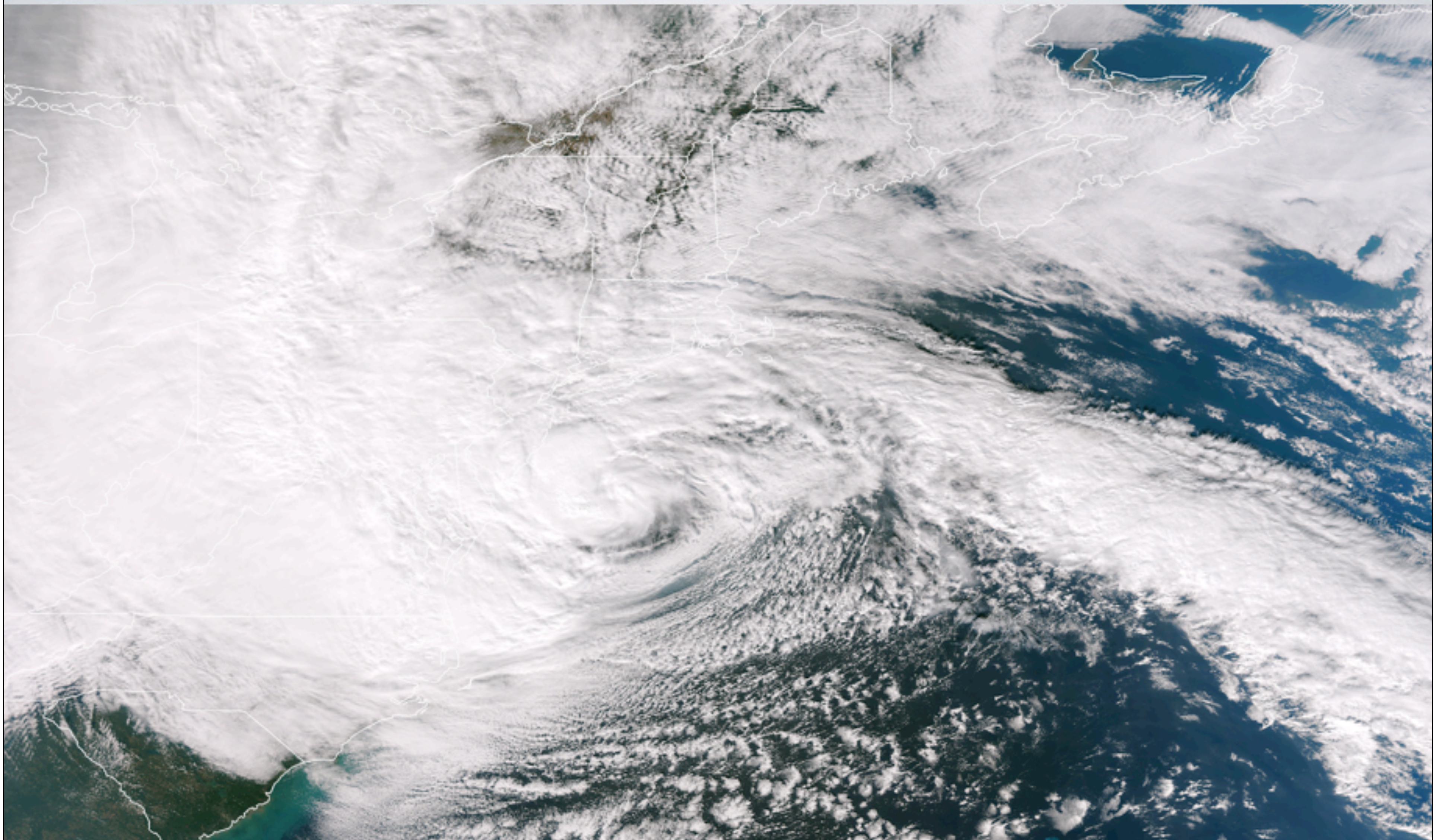


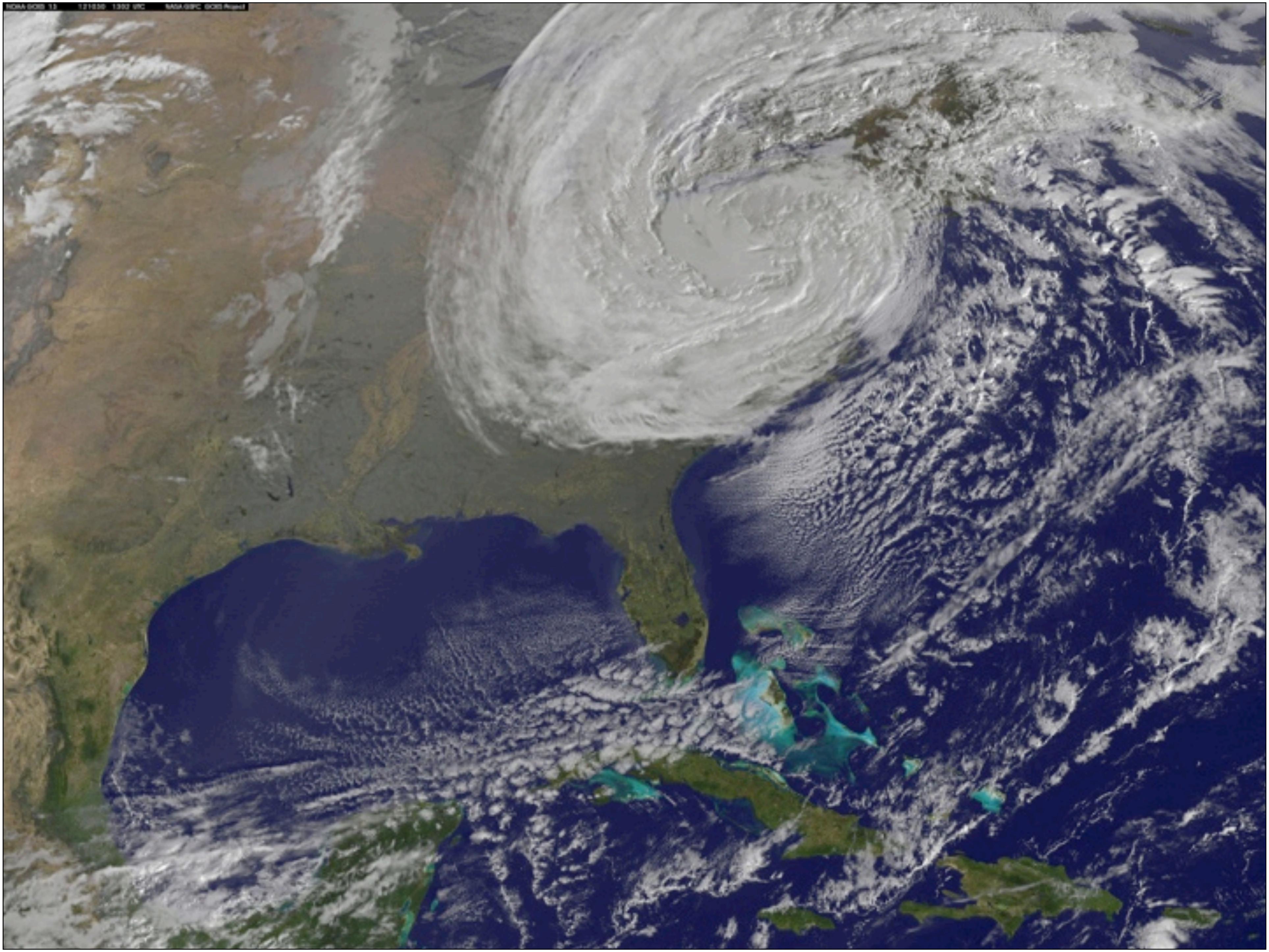
source: gapminder.org



HURRICANE SANDY 2012

HURRICANE SANDY OCTOBER 29, 2012





SOME OTHER EXAMPLES FROM 2012

- Spring 2012 saw the warmest March, third-warmest April and second-warmest May in history, and was approximately 5.2 degrees Fahrenheit above average overall.

- July was the hottest month ever recorded in the continental U.S., 3.3 degrees Fahrenheit above the 20th century average.

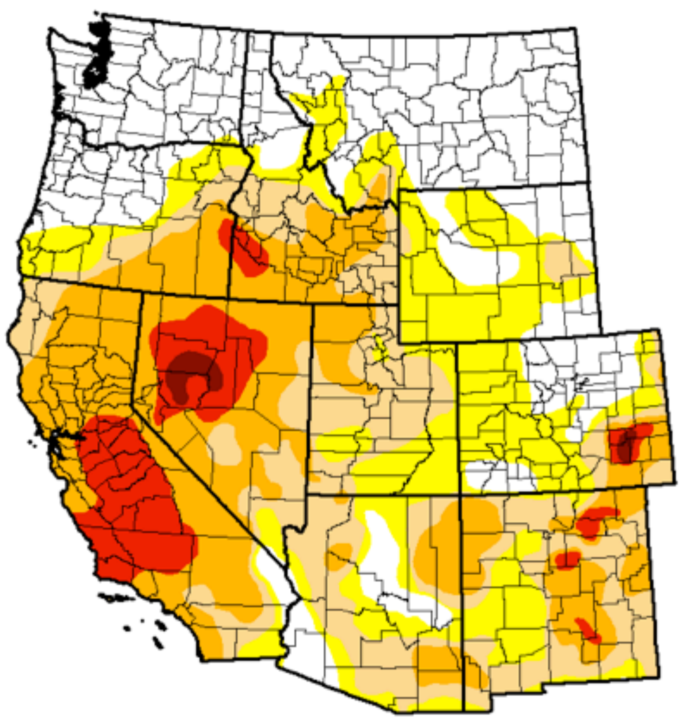
- The 2012 fire season 8.6 million acres – roughly the size of Connecticut and New Jersey combined – burned in the U.S.

Ref: http://thinkprogress.org/climate/issue/

DROUGHT IN THE MIDWEST

U.S. Drought Monitor

West



November 26, 2013

(Released Thursday, Nov. 28, 2013)

Valid 7 a.m. EST

Drought Conditions (Percent Area)

	None	D0-D4	D1-D4	D2-D4	D3-D4	D4
Current	29.00	71.00	49.99	30.86	7.56	0.63
Last Week 11/19/2013	27.36	72.64	53.20	32.23	7.56	0.63
3 Months Ago 8/27/2013	13.39	86.61	77.69	57.04	17.96	2.03
Start of Calendar Year 1/1/2013	24.39	75.61	69.31	45.04	18.01	2.15
Start of Water Year 10/1/2013	25.25	74.75	58.96	34.18	5.57	0.63
One Year Ago 11/27/2012	23.13	76.87	55.50	30.34	8.98	0.14

Intensity:

- D0 Abnormally Dry
- D1 Moderate Drought
- D2 Severe Drought
- D3 Extreme Drought
- D4 Exceptional Drought

The Drought Monitor focuses on broad-scale conditions. Local conditions may vary. See accompanying text summary for forecast statements.

Author:
Richard Heim
NCDC/NOAA

http://droughtmonitor.unl.edu/

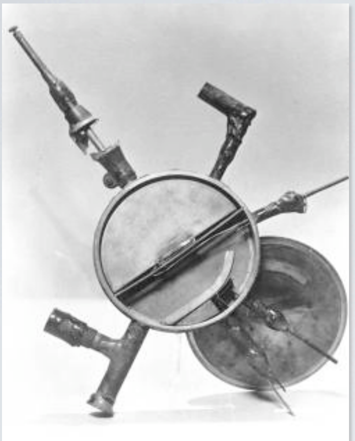
As of September, 64 percent of the continental U.S. is experiencing drought, with August and September 2012 comparable to the worst months of the 1930s Dust Bowl.

SEVERE WEATHER ALSO A CONCERN FOR CALIFORNIA

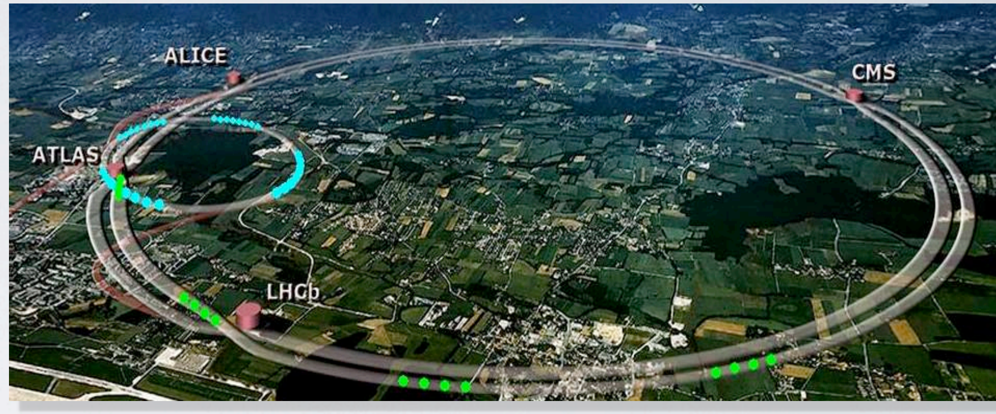
PART II

MATHEMATICS AND COMPUTERS TO THE RESCUE

Experiments vs. Computational Science



75,000 increase



4.5 inches diameter

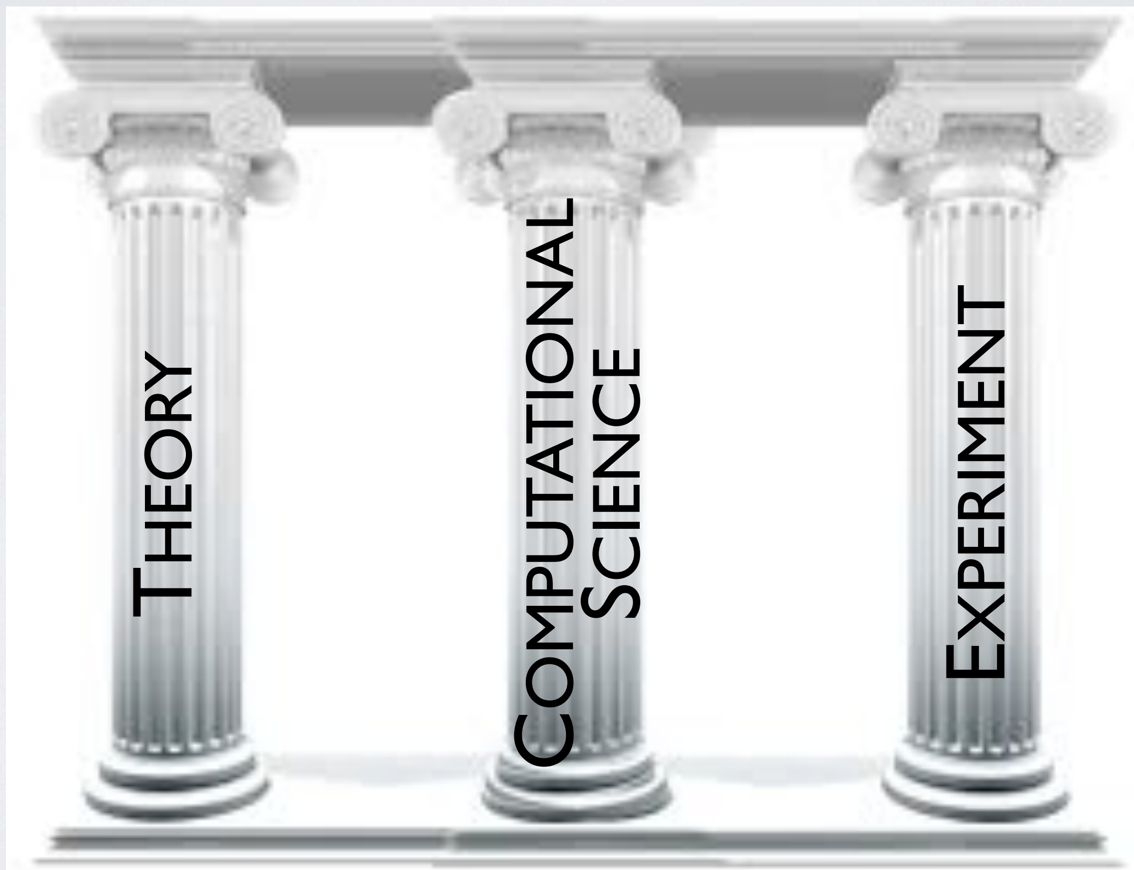
27 km circumference, $4B US

500 Million increase

400 operations/s, $500K

200 Billion operations/s, $400

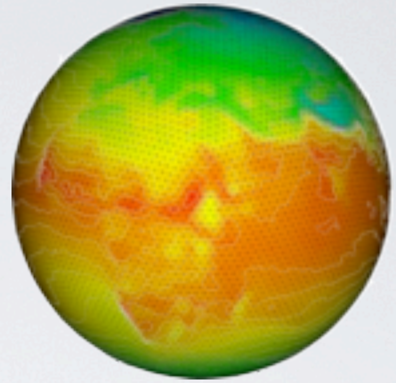
COMPUTATIONAL SCIENCE IS NOW CONSIDERED THIRD PILLAR OF SCIENCE



Unprecedented Progress

Energy Efficiency

Tools for predicting building energy use



Earth Systems

Computer models for predicting extreme events

Energy Storage

Understanding and designing next-generation batteries

Combustion

Understanding the dispersion of pollutants in the environment.

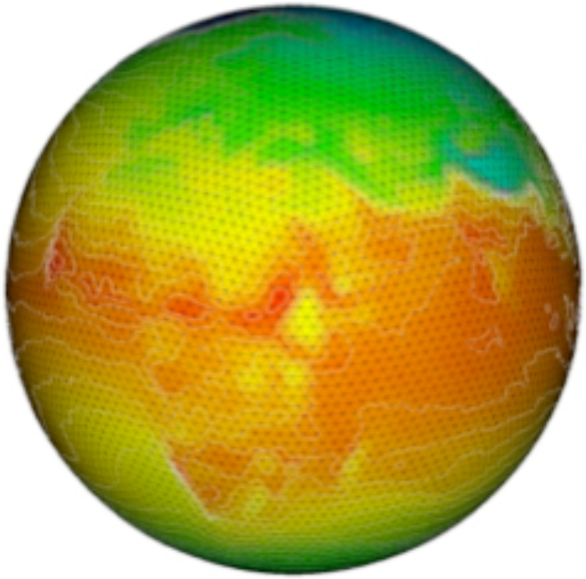
Biofuels

Simulation models for understanding bottlenecks to economical biofuels

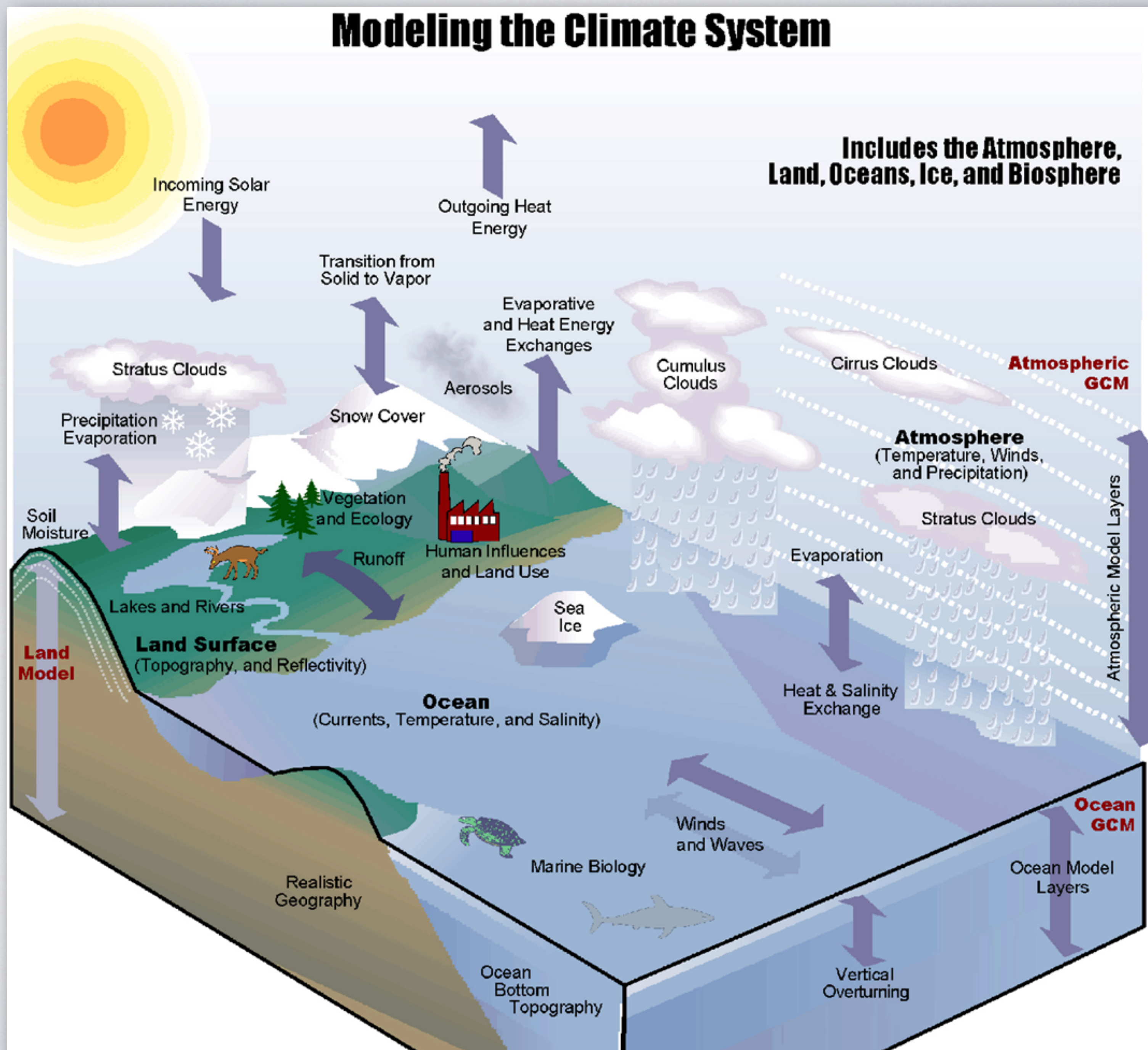
Nano Science

Predicting properties of next-generation photovoltaic solar cell materials.

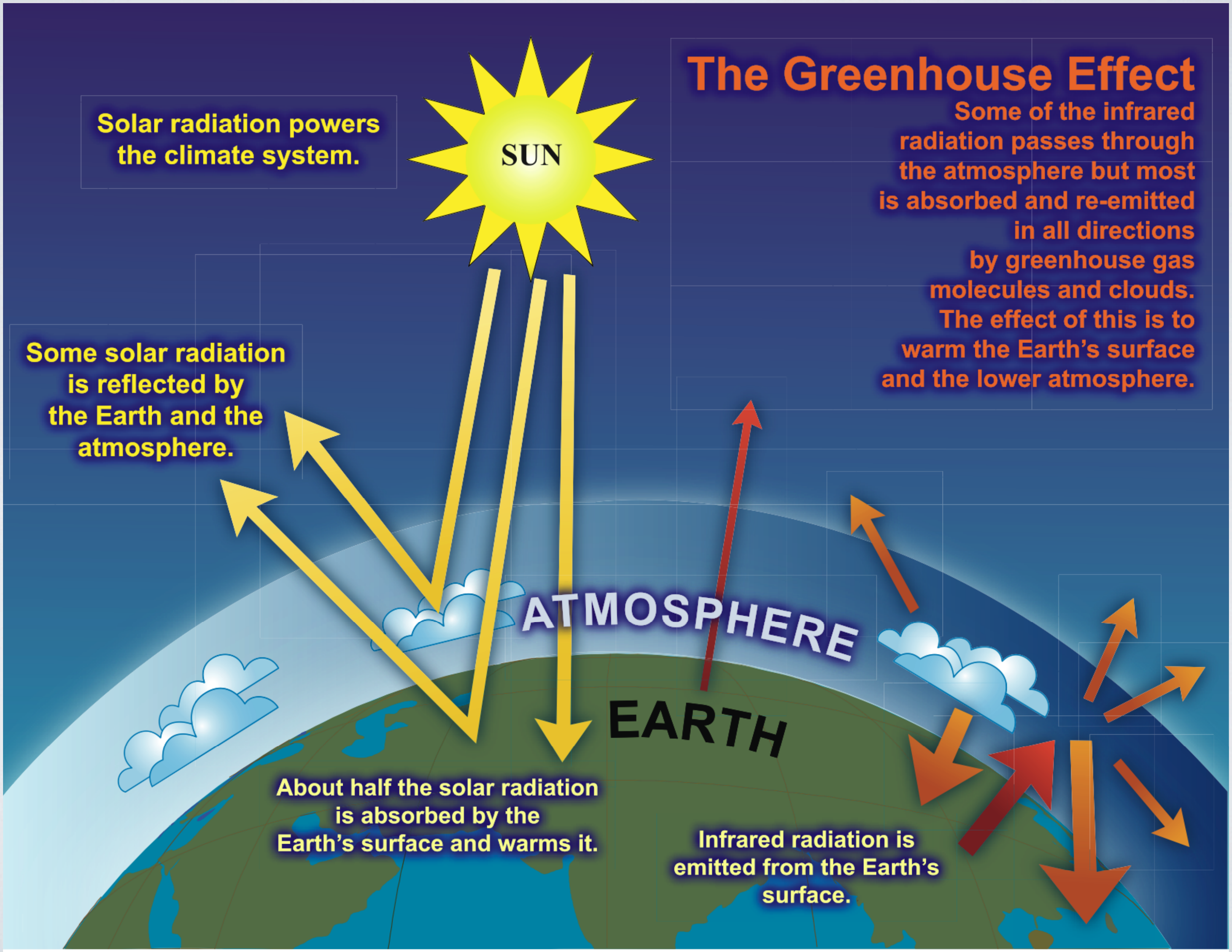
Images courtesy of Lawrence Berkeley National Laboratory



Climate Modeling

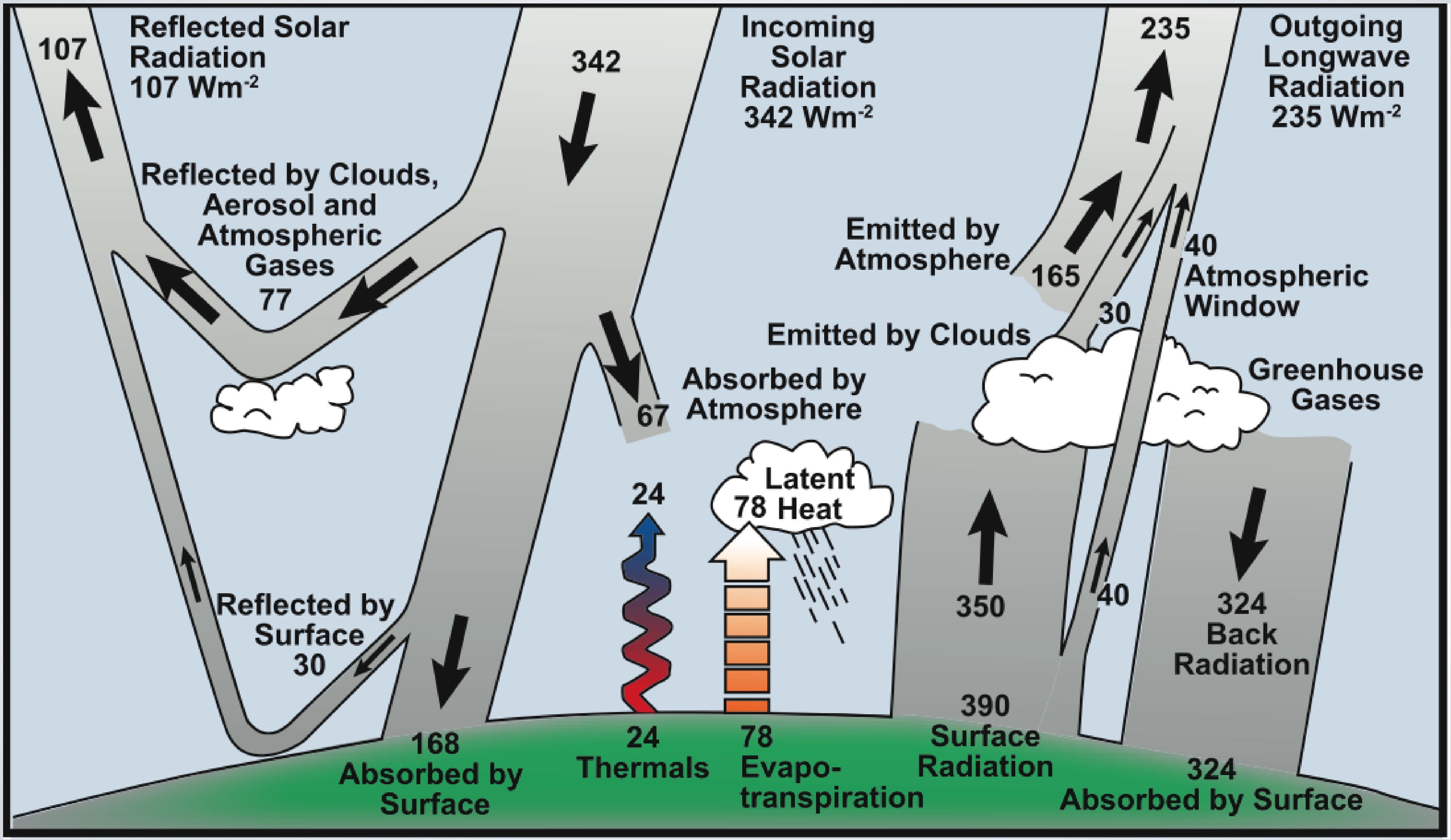

Modeling the Climate System
Includes the Atmosphere, Land, Oceans, Ice, and Biosphere
Incoming Solar Energy
Outgoing Heat Energy
Transition from Solid to Vapor
Evaporative and Heat Energy Exchanges
Stratus Clouds
Cumulus Clouds
Cirrus Clouds
Atmospheric GCM
Aerosols
Snow Cover
Precipitation Evaporation
Atmosphere
(Temperature, Winds, and Precipitation)
Vegetation and Ecology
Stratus Clouds
Soil Moisture
Runoff
Human Influences and Land Use
Evaporation
Atmospheric Model Layers
Lakes and Rivers
Sea Ice
Land Model
Land Surface
(Topography, and Reflectivity)
Heat & Salinity Exchange
Ocean
(Currents, Temperature, and Salinity)
Ocean GCM
Winds and Waves
Marine Biology
Ocean Model Layers
Realistic Geography
Ocean Bottom Topography
Vertical Overturning

GREENHOUSE EFFECT



ATMOSPHERE ENERGY BALANCE

342 = 107 + 235



FIRST MENTION OF GREENHOUSE EFFECT (1824)

- Fourier developed mathematical theory for the temperature of the terrestrial globe

- "The temperature [of the Earth] can be augmented by the interposition of the atmosphere, because heat in the state of light finds less resistance in penetrating the air, than in repassing into the air when converted into non-luminous heat" (1824)

FOURIER

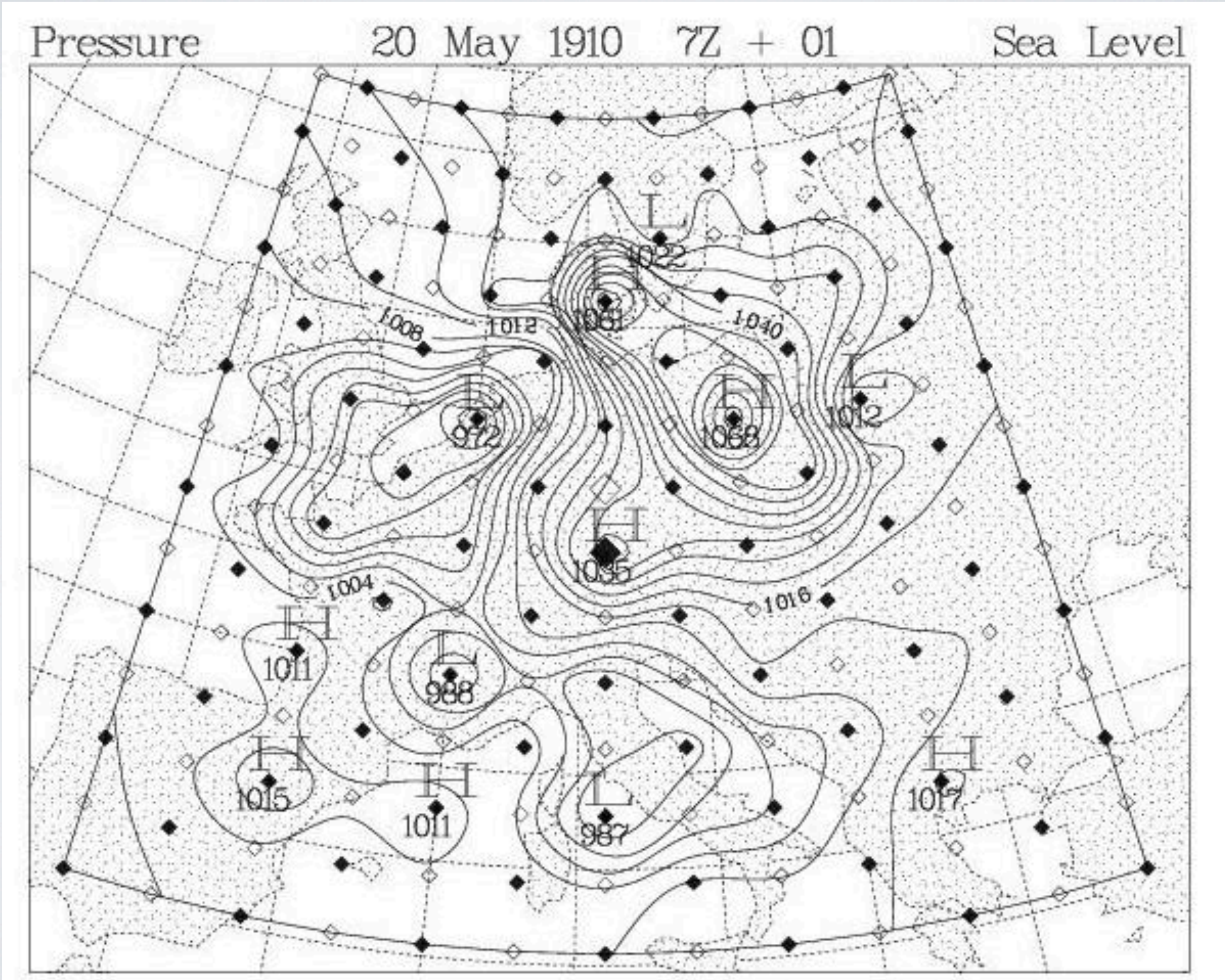
NUMERICAL WEATHER FORECASTING

- British mathematician Lewis Fry Richardson proposed numerical weather forecasting in 1922
- Computed 1 day weather forecast over a period of 6 weeks, while working as the driver of a Quaker ambulance unit in northern France.
- Sadly, first calculations were unsuccessful, due to numerical problems

LEWIS FRY RICHARDSON

Fascinating talk by Peter Lynch (University College Dublin) can be found at:
http://www.ncep.noaa.gov/nwp50/Presentations/Tue_06_15_04/Session_1/Lynch_NWP50.pdf

RICHARDSON'S COMPUTATION



PRIMITIVE EQUATIONS FOR ATMOSPHERE

$$\frac{du}{dt} - \left(f + u\frac{\tan\phi}{a}\right)v = -\frac{1}{a\cos\phi}\frac{1}{\rho}\frac{\partial p}{\partial \lambda} + F_\lambda$$

$$\frac{dv}{dt} + \left(f + u\frac{\tan\phi}{a}\right)u = -\frac{1}{\rho a}\frac{\partial p}{\partial \phi} + F_\phi$$

$$g = -\frac{1}{\rho}\frac{\partial p}{\partial z}$$

Conservation of momentum

$$\frac{\partial \rho}{\partial t} = -\frac{1}{a\cos\phi}\left[\frac{\partial}{\partial \lambda}(\rho u) + \frac{\partial}{\partial \phi}(\rho v\cos\phi)\right] - \frac{\partial}{\partial z}(\rho w)$$

Conservation of mass

$$C_p\frac{dT}{dt} - \frac{1}{\rho}\frac{dp}{dt} = Q$$

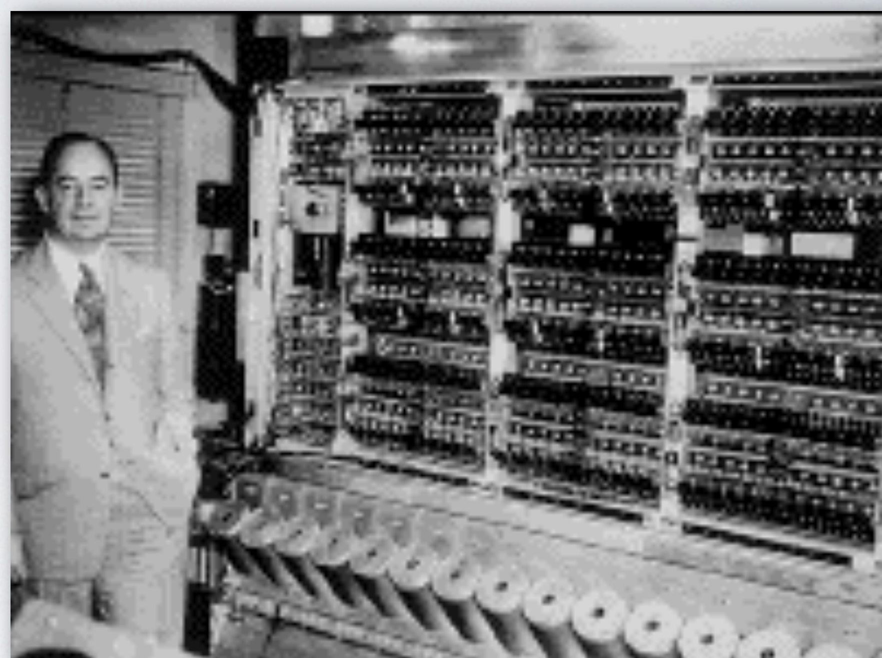
Conservation of energy

$$p = \rho R T$$

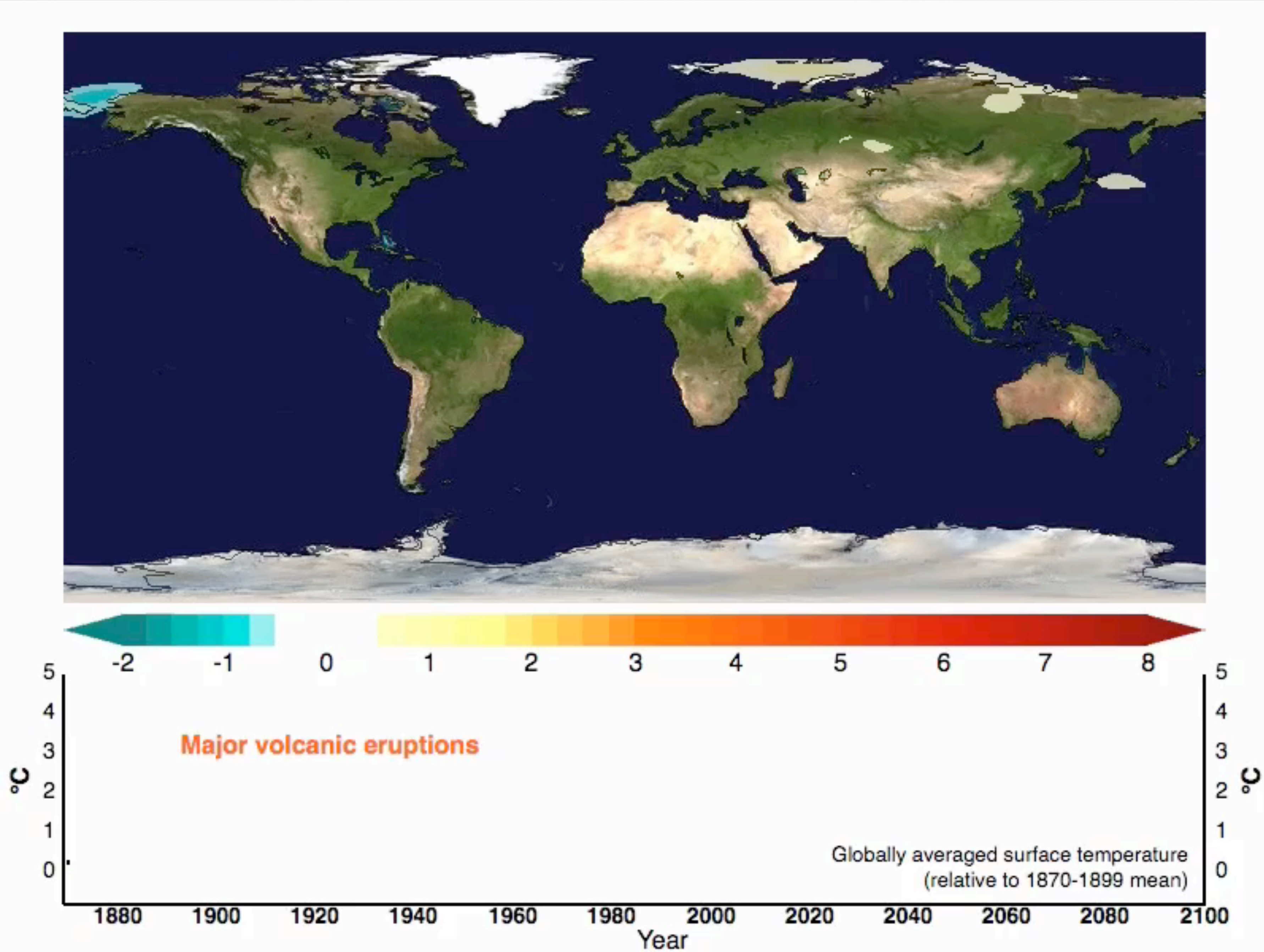
Equation of state

JOHN VON NEUMANN'S METEOROLOGY PROJECT

- Recognized numerical weather forecasting as a problem of great importance
- In collaboration with Charney and Fjortoft, they completed the first numerical computer forecast in 1950
- Used ENIAC, first multipurpose electronic digital computer
- Each 24 hour forecast took 24 hours to compute

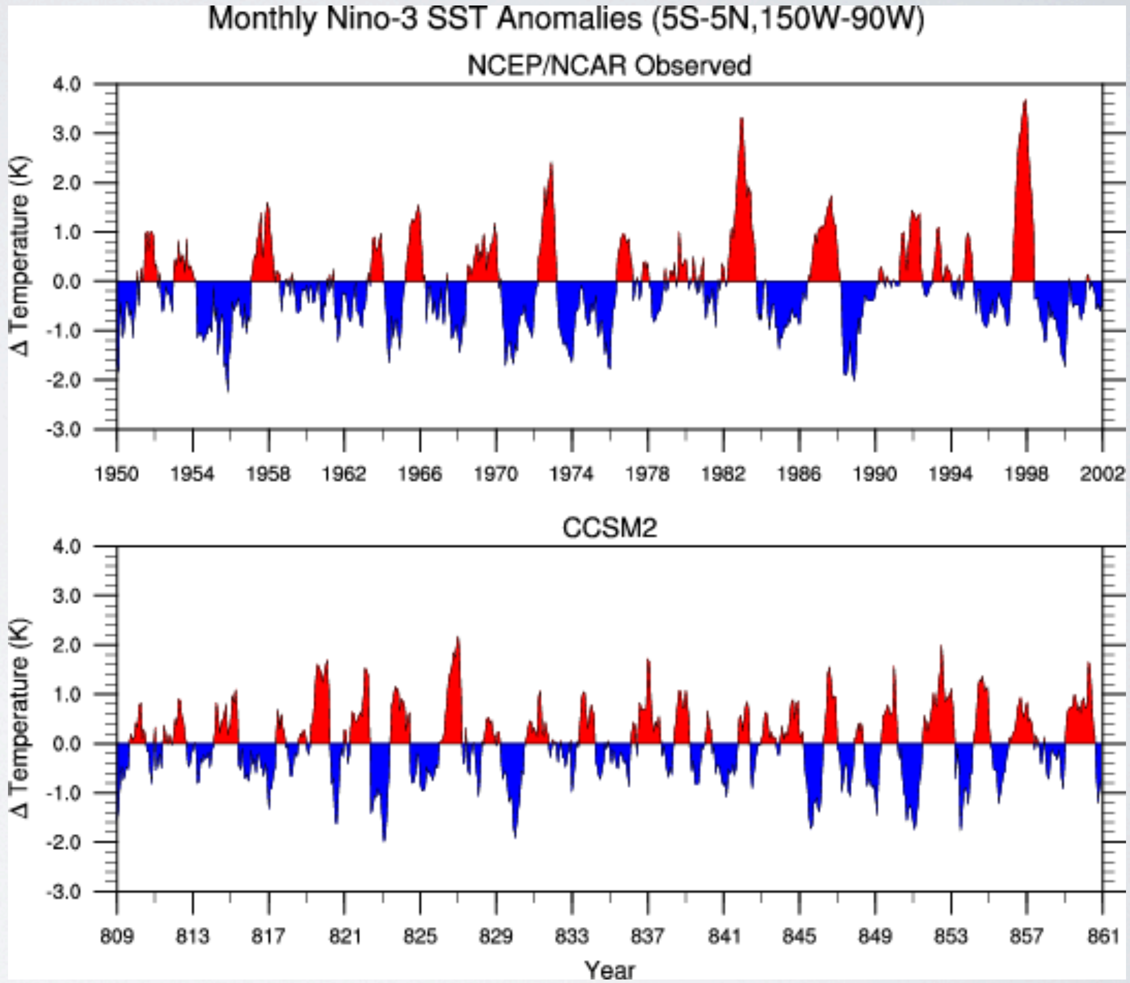


"If people do not believe that mathematics is simple, it is only because they do not realize how complicated life is."


-2
-1
0
1
2
3
4
5
6
7
8
°C
5
4
3
2
1
0
Major volcanic eruptions
Globally averaged surface temperature
(relative to 1870-1899 mean)
1880
1900
1920
1940
1960
1980
2000
2020
2040
2060
2080
2100
Year

1000 YEAR SIMULATIONS NOW POSSIBLE

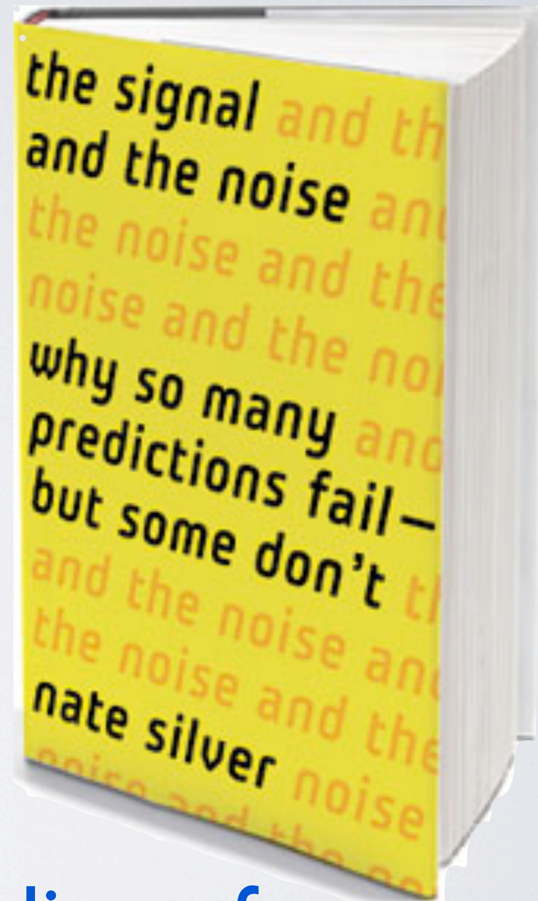
- A 1000-year simulation demonstrates the ability of models to produce a long-term, stable representation of the earth's climate.
- Used more than 1 million processor hours over several months



Warren Washington and Jerry Meehl, National Center for Atmospheric Research; Bert Semtner, Naval Postgraduate School; John Weatherly, U.S. Army Cold Regions Research and Engineering Lab Laboratory.

HOW CONFIDENT CAN WE BE IN OUR MATH & COMPUTER MODELS?

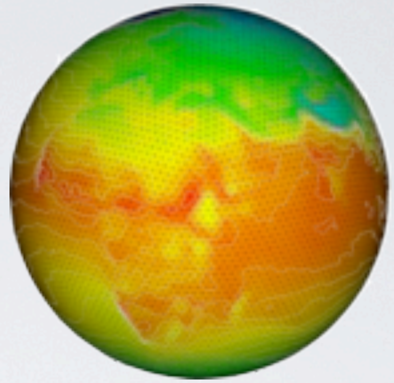
- There are uncertainties in the computer models
- There are uncertainties in the input data
- Math models are incomplete representations at best



Must have an understanding of probability and statistics

Unprecedented Progress

Energy Efficiency
Tools for predicting building energy use



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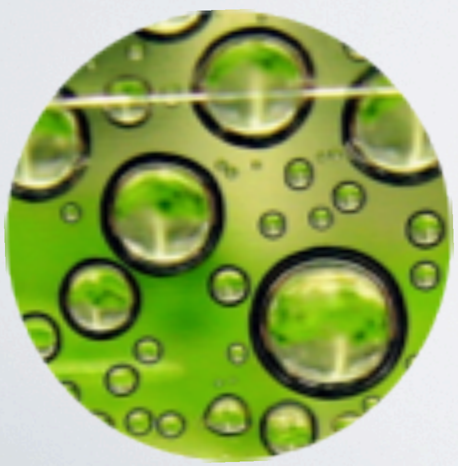
Computer models for predicting extreme events

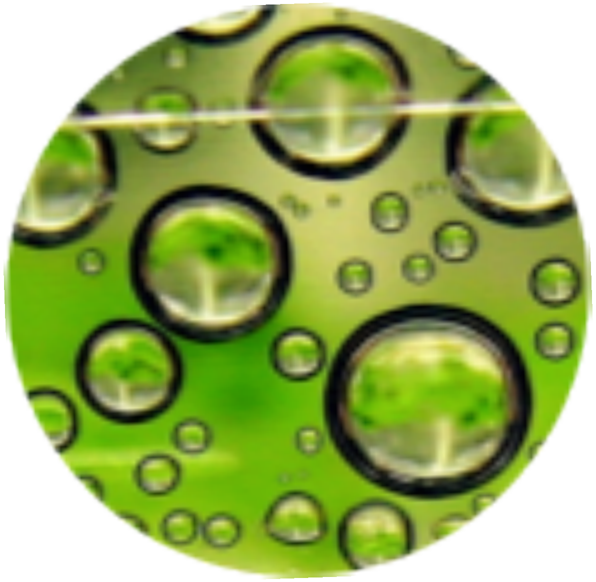
Energy Storage
Understanding and designing next-generation batteries

Combustion
Understanding the dispersion of pollutants in the environment.



Biofuels
Simulation models for understanding bottlenecks to economical biofuels

Nano Science
Predicting properties of next-generation photovoltaic solar cell materials.

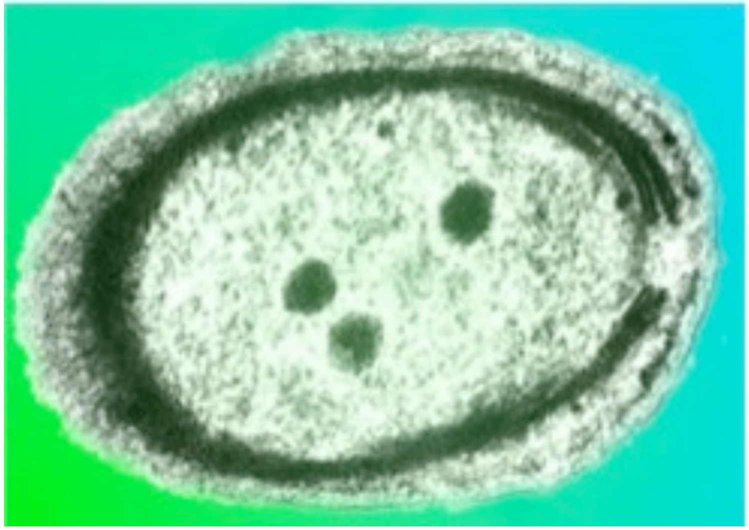


Biofuels

Simulation models for understanding bottlenecks to economical biofuels

Biofuels

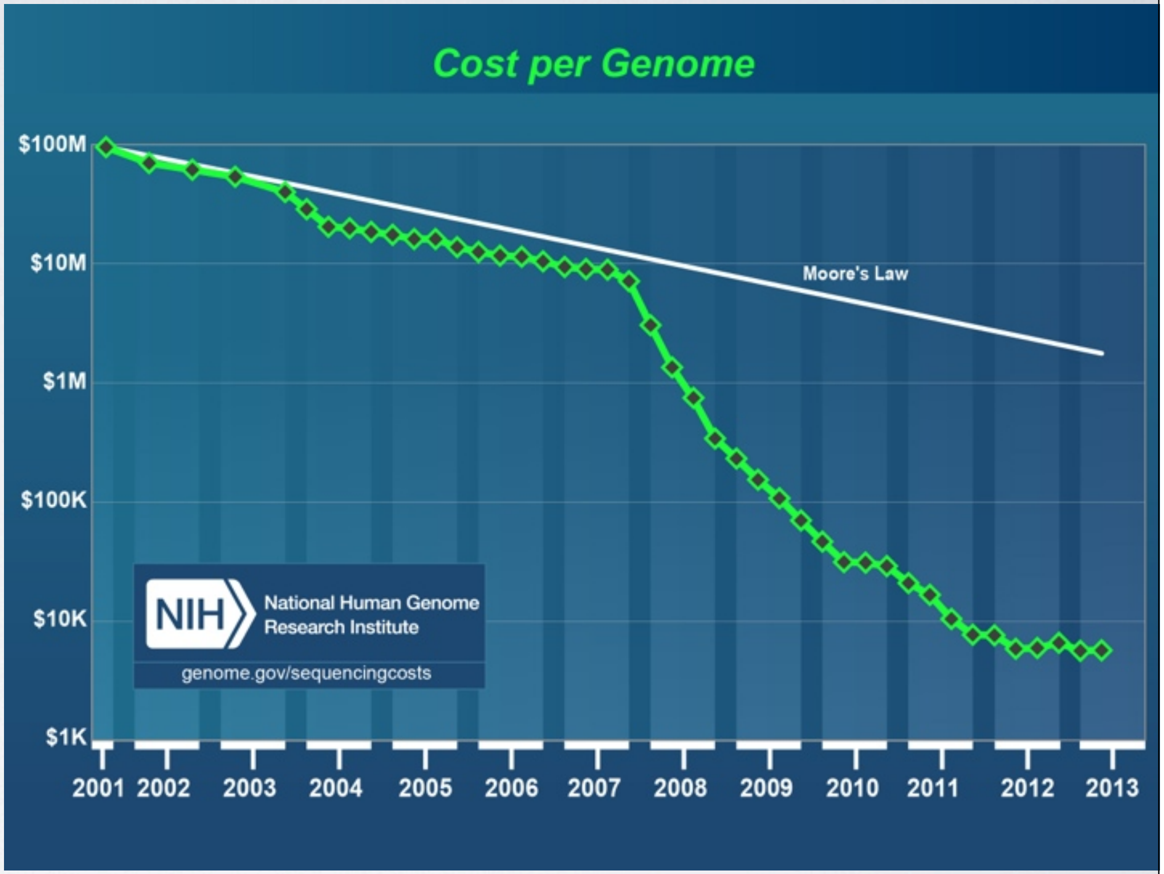
PHOTOGRAPH COURTESY USDA-ARS VIA PNAS



- Plants have evolved to be resistant to physical and chemical attack
- How do bacteria remove carbon from the atmosphere?
- If we can understand plant genomics better could we design better biofuels?

Data Enabled Science

- Many scientific problems are now rate-limited by access to and analysis of data
- Genome sequencing is outpacing computing and algorithms
- High school students are now accessing and using genomic data for studies
- $1000 genome will soon be here

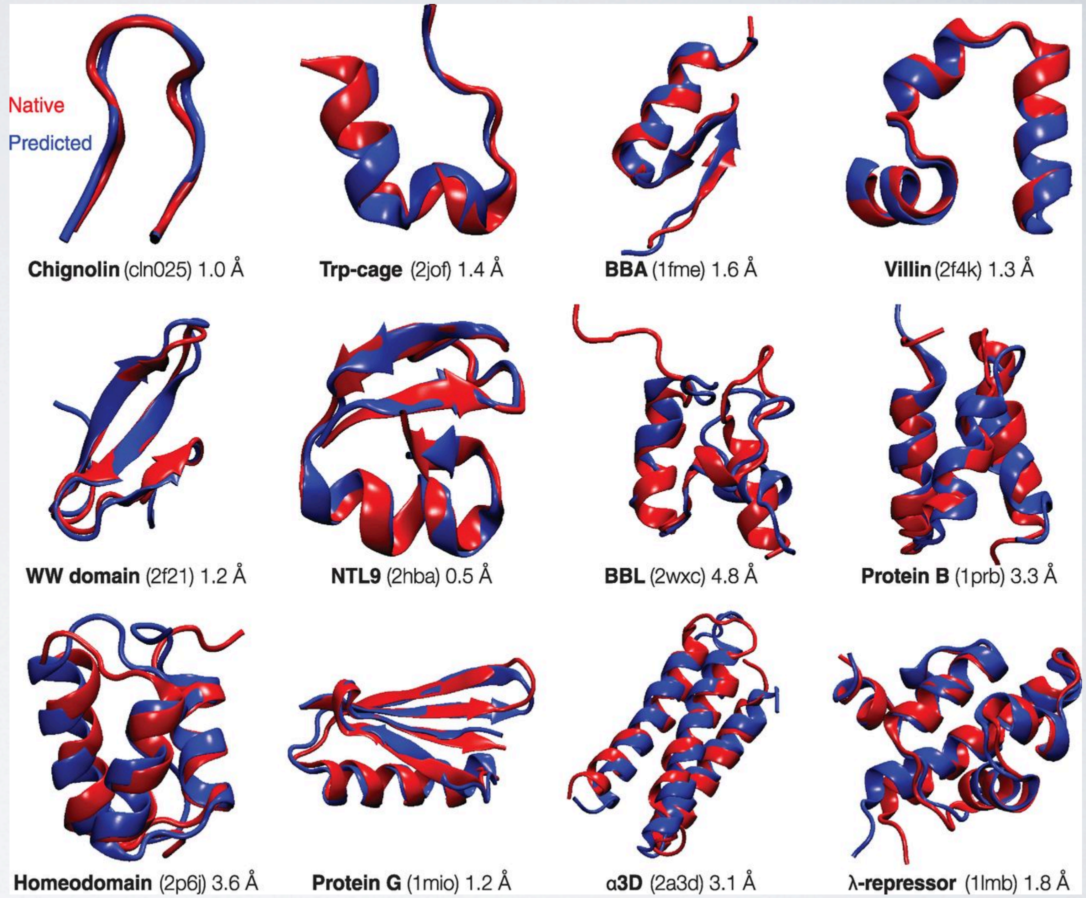


Wetterstrand KA. DNA Sequencing Costs: Data from the NHGRI Genome Sequencing Program (GSP) Available at: http://www.genome.gov/sequencingcosts/

On the Future of Genomic Data, Scott D. Kahn, Science **331**, 728 (2011)

Protein Folding problem

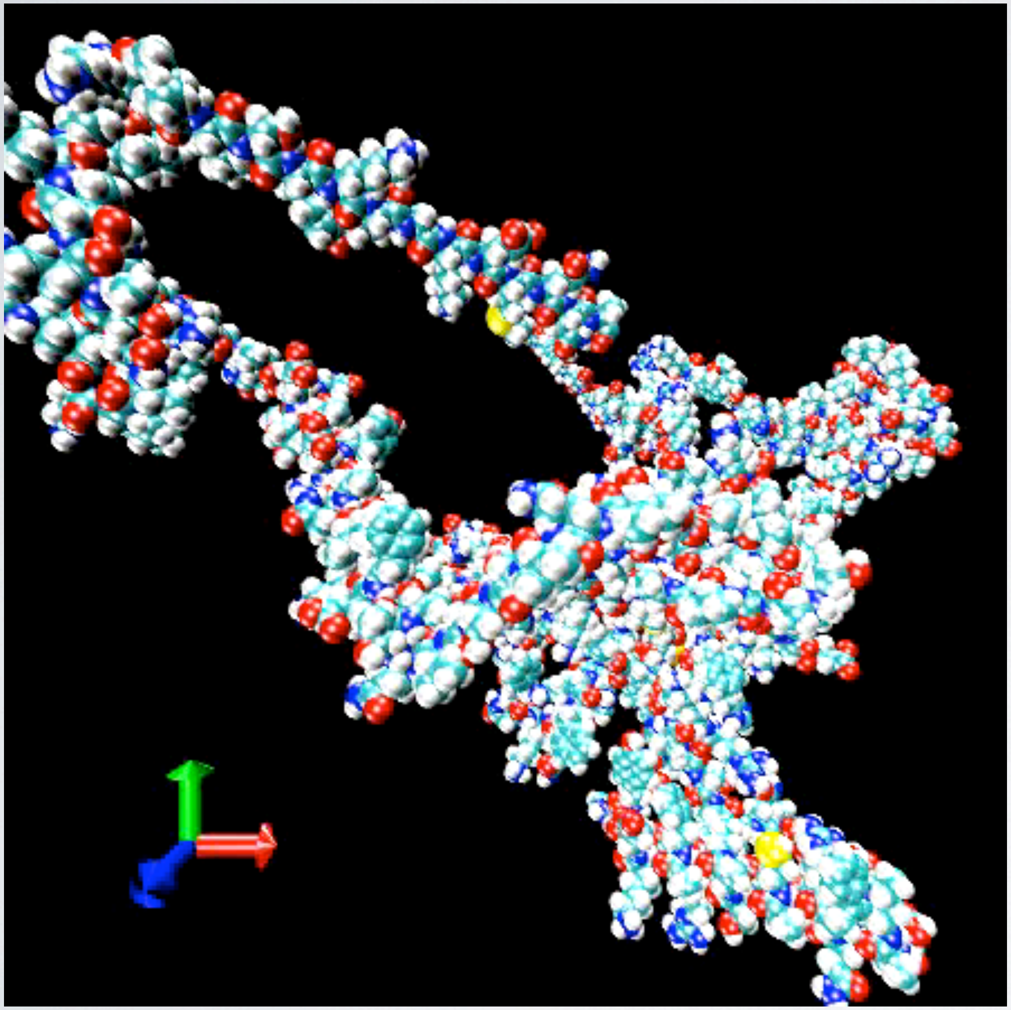
- Genome sequence is only the start
- The 3D shape of a protein determines its function
- One of the grand scientific challenges.



K A Dill, and J L MacCallum Science 2012;338:1042-1046

Science AAAS

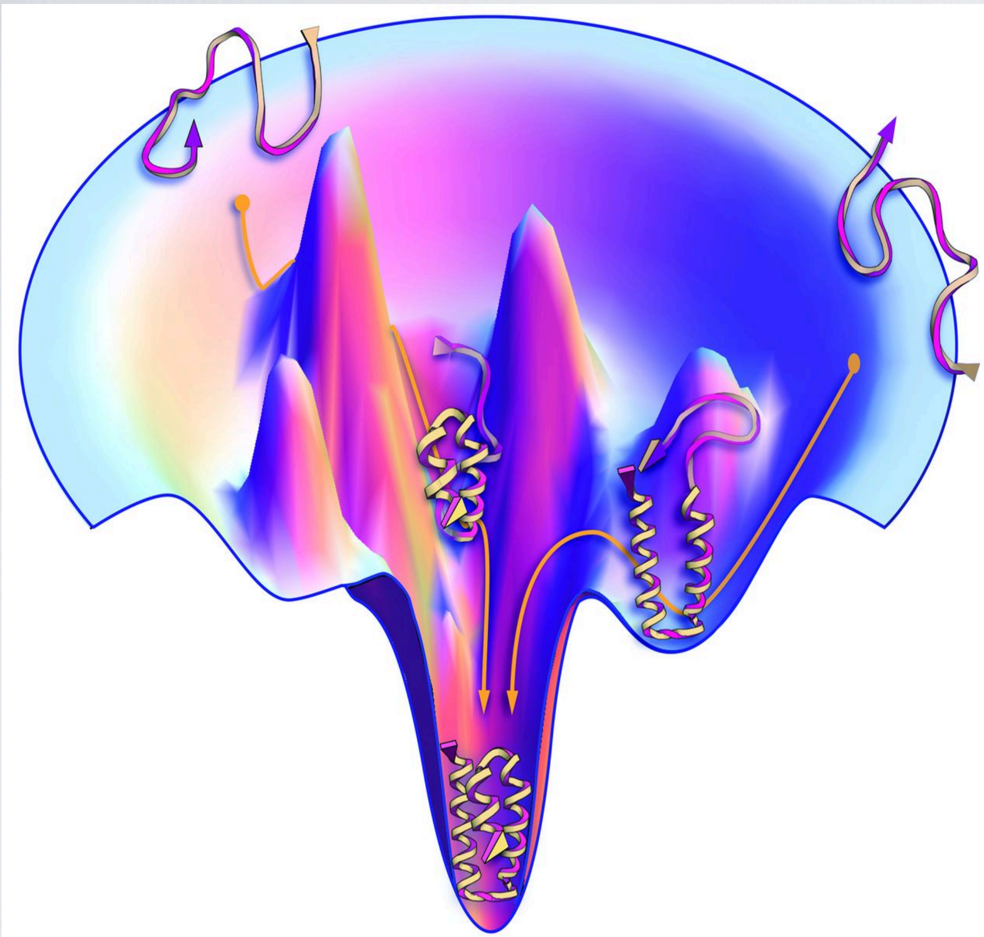
Protein Folding used in drug design



- A single new drug may cost over $800 million and take over 10 years to develop
- Computer simulations can be used to predict new drugs
- Mathematical models can compute the energy of a molecule

Juan Meza, Ricardo Oliva, Scientific Computing, LBNL

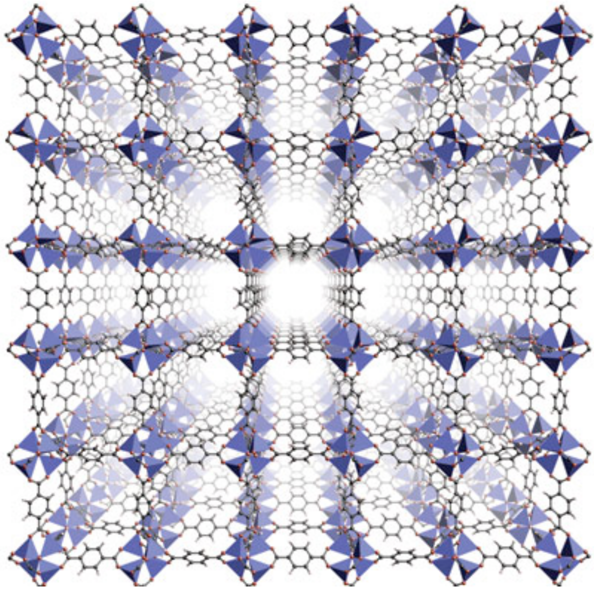
Protein Folding Unsolved Problems

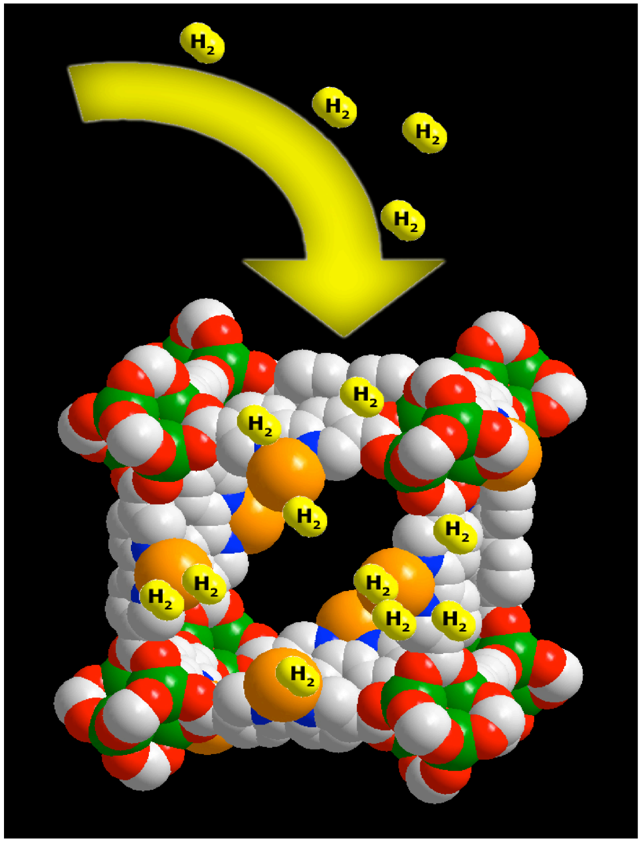


Dill and MacCallum, Science 338, 1042(2012)

- Cannot consistently predict structures with high accuracy
- Don't have understanding of folding routes
- Don't have algorithms for computing binding affinities of drugs and small molecules to proteins

Many, many more applications





SUMMARY

- Unprecedented increases in math and computational power have opened new opportunities in energy, environment, biology

- Many unsolved problems waiting to be studied

- We need many more people with new ideas working on these problems

So If Someone Asks You Why You're Studying Math?

I'm Going To Help Save The World!


TRASH