Computational Math and Science

How Mathematics Will Help Save The World

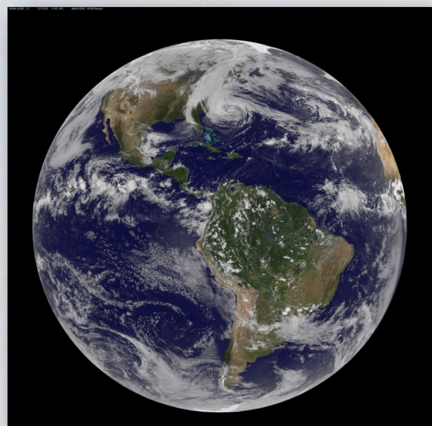
Juan Meza

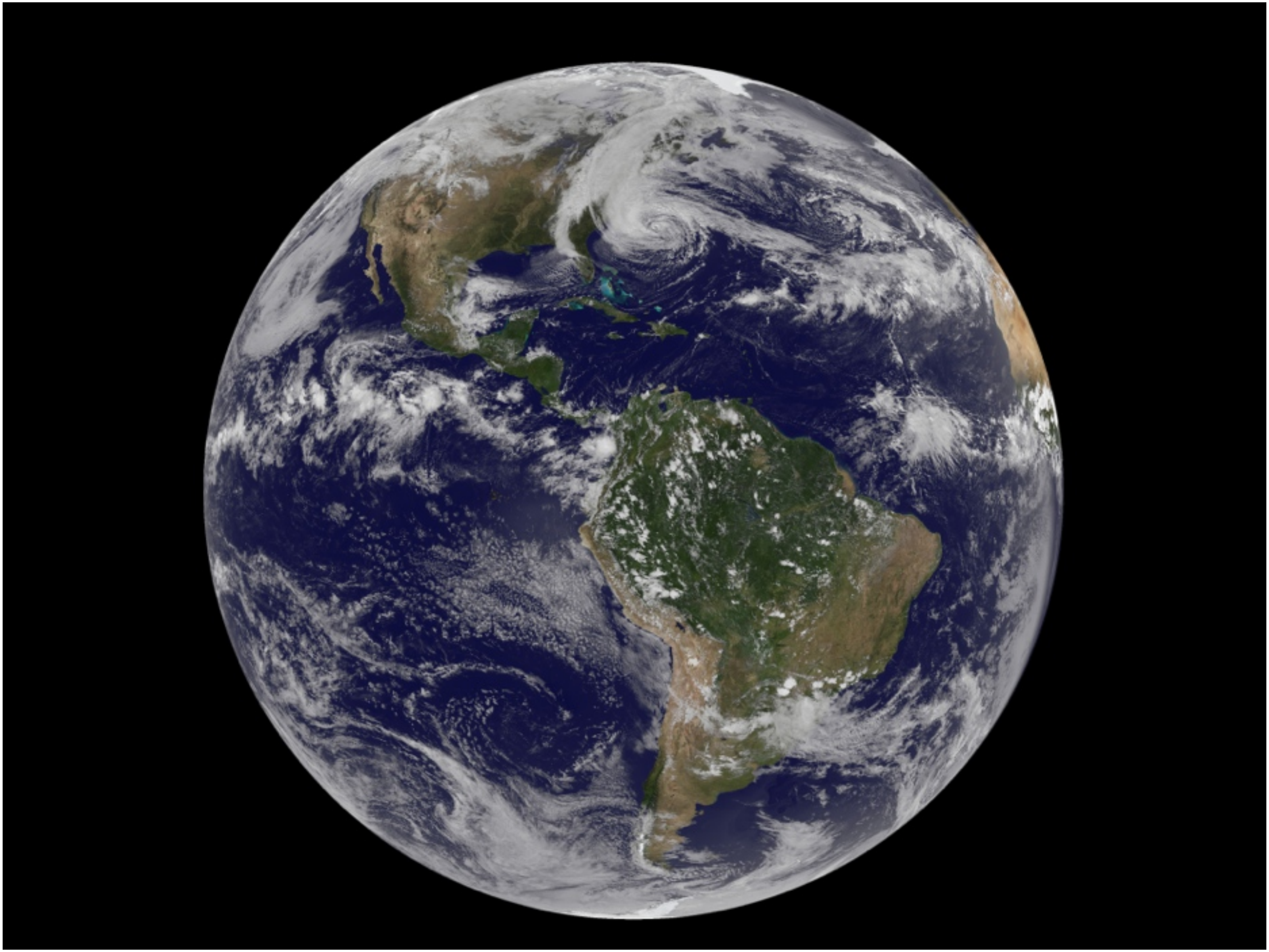
Professor Applied Mathematics

Dean, School of Natural Sciences, UC Merced

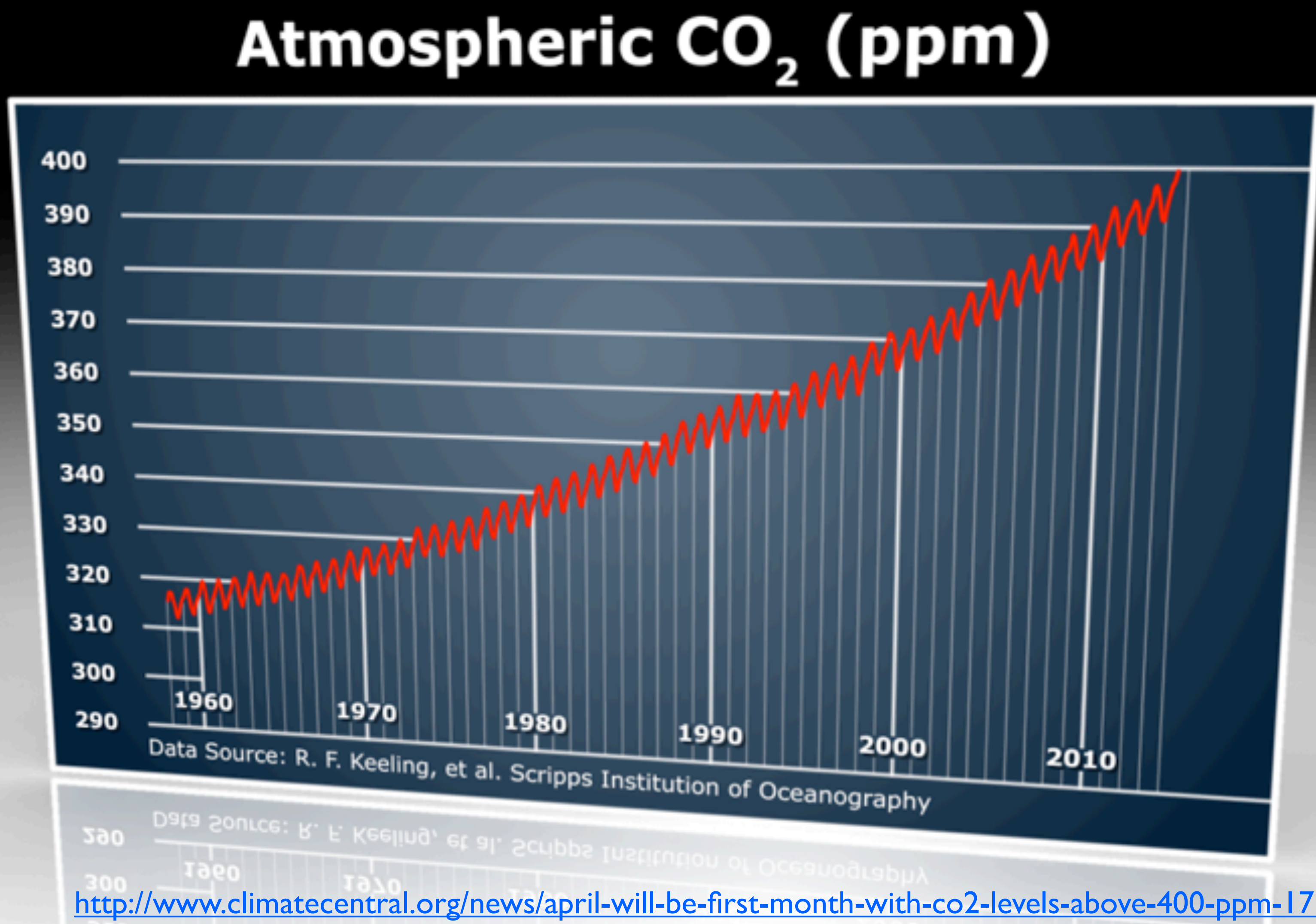
source: gapminder.org

Let’s do an experiment

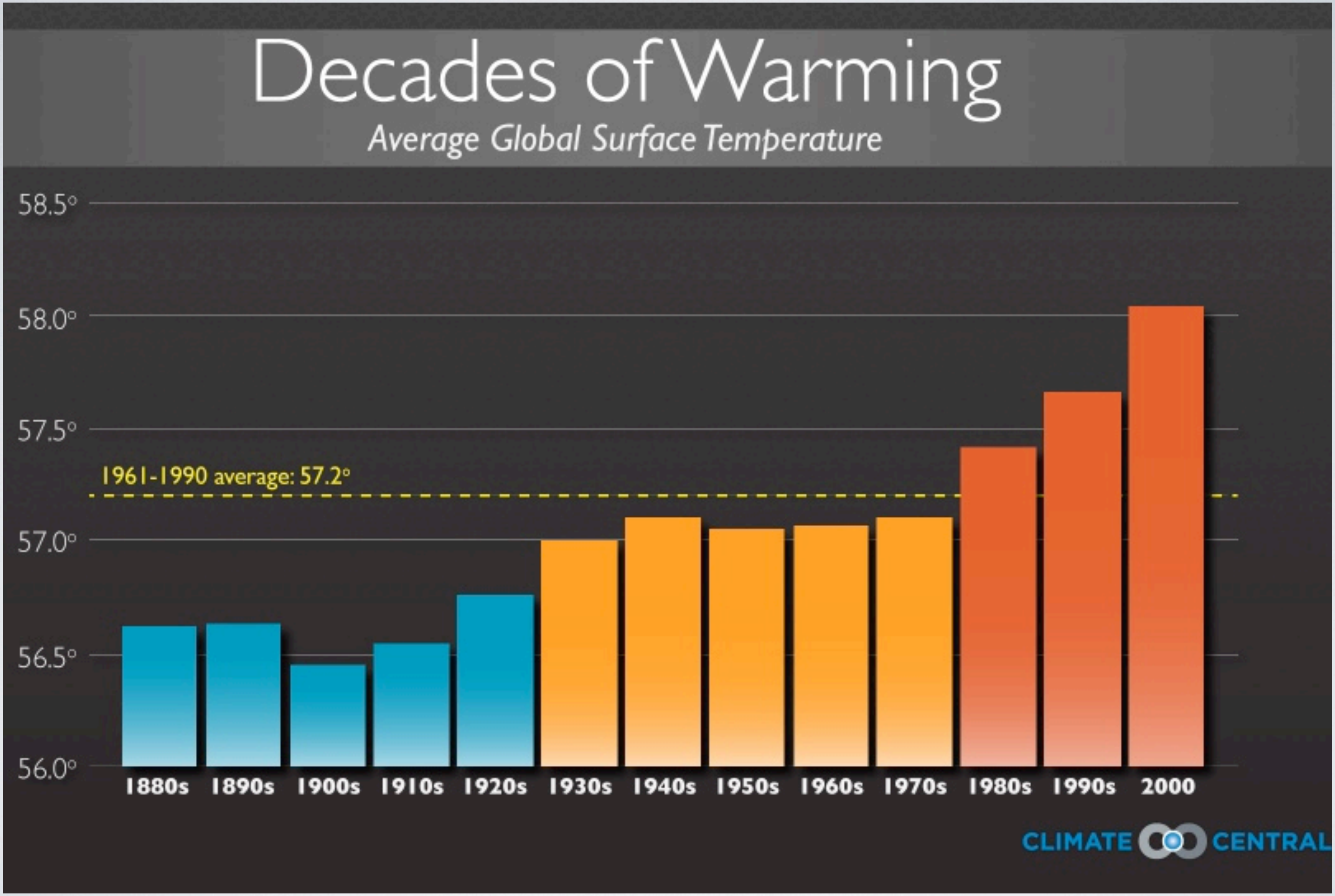
 +  = ?



April Will Be First Month With CO2 Levels

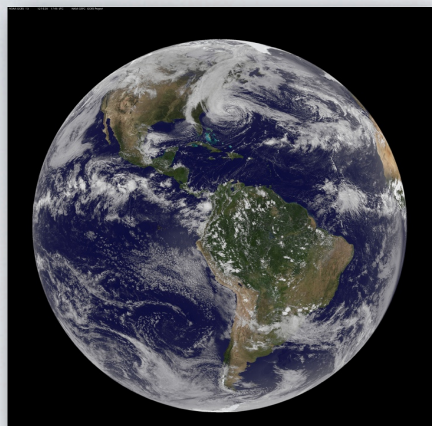


http://www.climatecentral.org/news/april-will-be-first-month-with-co2-levels-above-400-ppm-17331



Decades of Warming
Average Global Surface Temperature
58.5°
58.0°
57.5°
57.0°
56.5°
56.0°
1961-1990 average: 57.2°
1880s
1890s
1900s
1910s
1920s
1930s
1940s
1950s
1960s
1970s
1980s
1990s
2000
CLIMATE CENTRAL

LET'S DO AN EXPERIMENT



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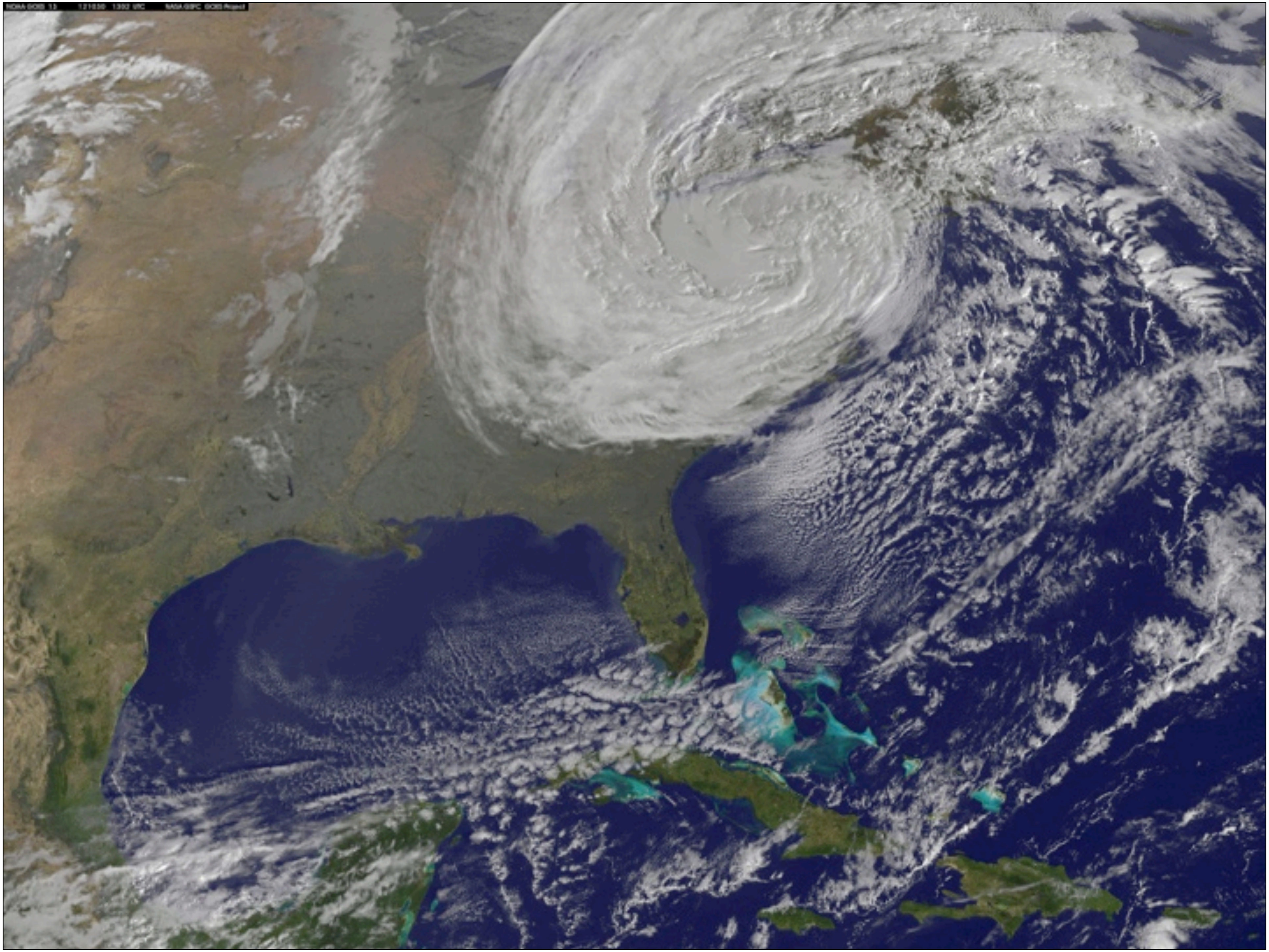
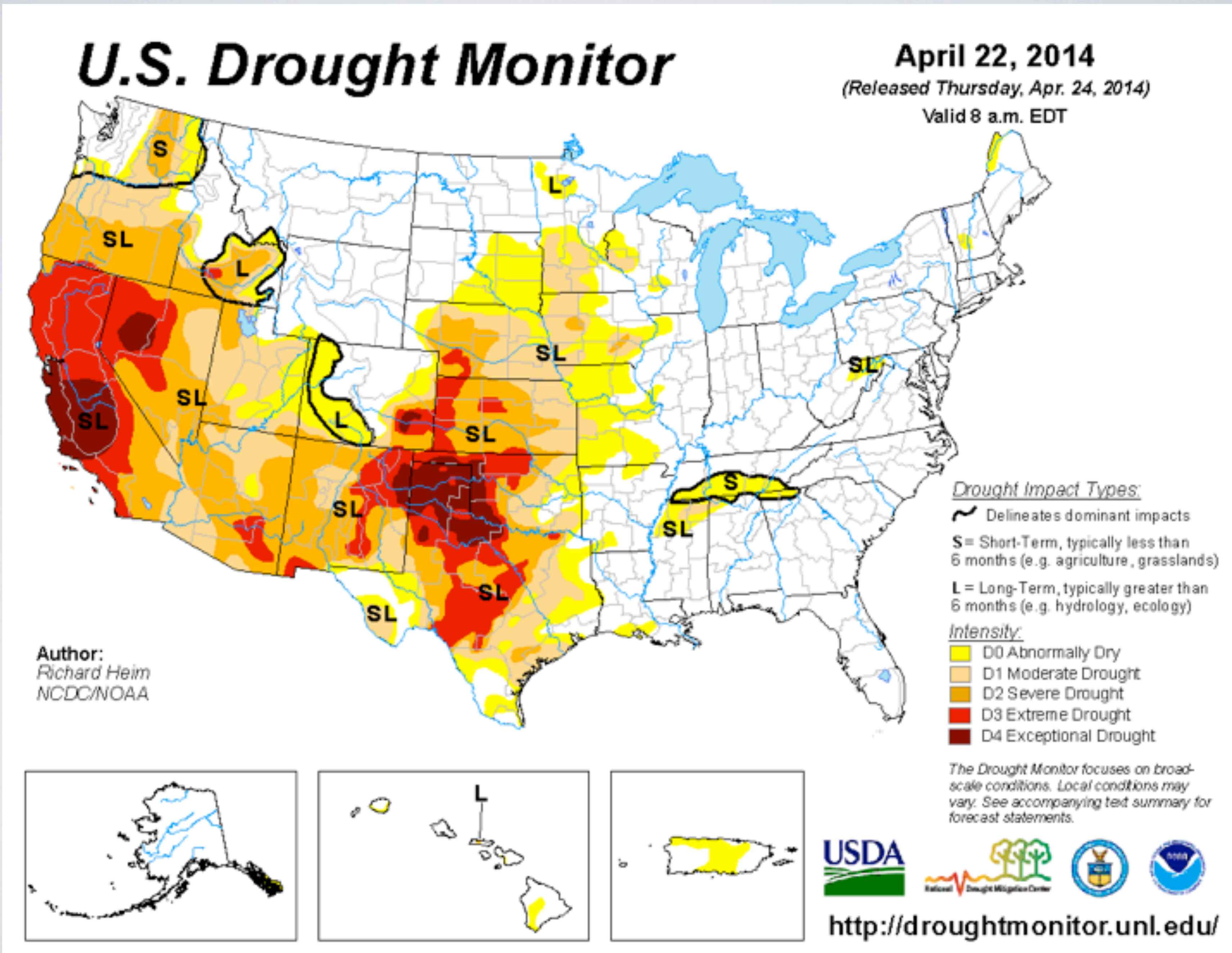
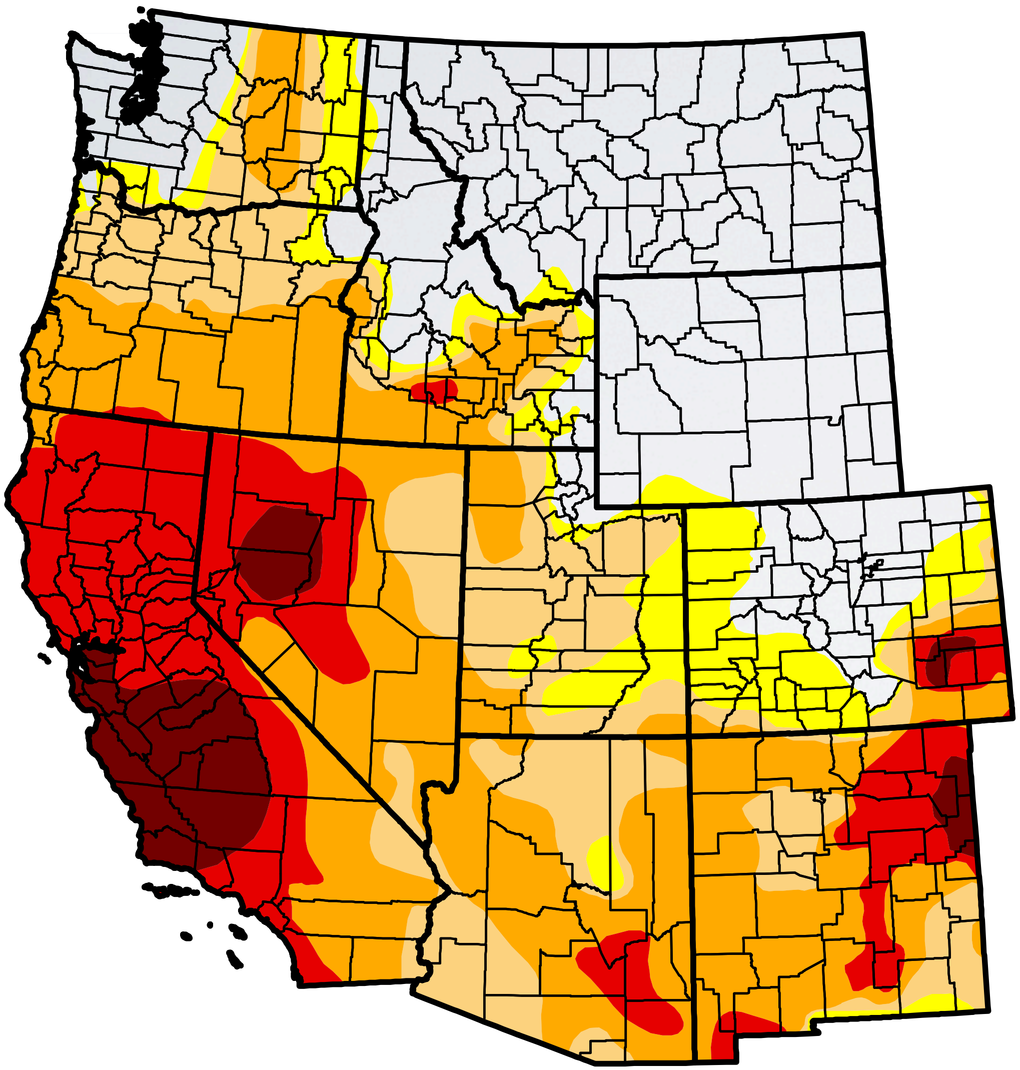



U.S. Drought Monitor
April 22, 2014
(Released Thursday, Apr. 24, 2014)
Valid 8 a.m. EDT
S
L
SL
Drought Impact Types:
Delineates dominant impacts
S = Short-Term, typically less than 6 months (e.g. agriculture, grasslands)
L = Long-Term, typically greater than 6 months (e.g. hydrology, ecology)
Intensity:
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
USDA
http://droughtmonitor.unl.edu/

U.S. Drought Monitor
West

April 22, 2014
(Released Thursday, Apr. 24, 2014)
Valid 8 a.m. EDT



Drought Conditions (Percent Area)

	None	D0-D4	D1-D4	D2-D4	D3-D4	D4
Current	30.11	69.89	61.61	45.09	17.93	4.61
Last Week *4/15/2014*	30.08	69.92	60.68	43.68	16.06	4.05
3 Months Ago *1/21/2014*	18.74	81.26	60.81	36.99	13.78	0.63
Start of Calendar Year *12/31/2013*	22.20	77.80	51.44	31.11	7.75	0.63
Start of Water Year *10/1/2013*	25.25	74.75	58.96	34.18	5.57	0.63
One Year Ago *4/23/2013*	20.28	79.72	66.00	43.41	16.10	1.87

Intensity:

- D0 Abnormally Dry
- D1 Moderate Drought
- D2 Severe Drought
- D3 Extreme Drought
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Author:
Richard Heim
NCDC/NOAA

http://droughtmonitor.unl.edu/

U.S. Drought Monitor
California

April 22, 2014
(Released Thursday, Apr. 24, 2014)
Valid 8 a.m. EDT

Drought Conditions (Percent Area)

	None	D0-D4	D1-D4	D2-D4	D3-D4	D4
Current	0.00	100.00	100.00	96.01	76.68	24.77
Last Week *4/15/2014*	0.00	100.00	99.80	95.21	68.76	23.49
3 Months Ago *1/21/2014*	1.43	98.57	94.18	89.91	62.71	0.00
Start of Calendar Year *12/31/2013*	2.61	97.39	94.25	87.53	27.59	0.00
Start of Water Year *10/1/2013*	2.63	97.37	95.95	84.12	11.36	0.00
One Year Ago *4/23/2013*	2.84	97.16	63.42	30.00	0.00	0.00

Intensity:

- D0 Abnormally Dry
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- D2 Severe Drought
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The Drought Monitor focuses on broad-scale conditions. Local conditions may vary. See accompanying text summary for forecast statements.

Author:
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NCDC/NOAA

USDA National Drought Mitigation Center

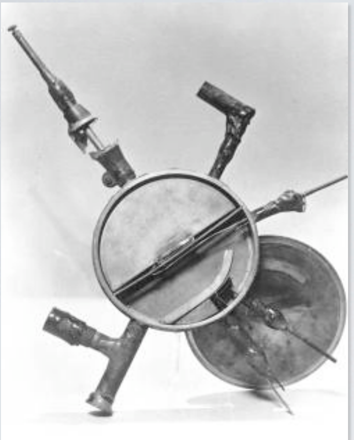
http://droughtmonitor.unl.edu/

http://ngm.nationalgeographic.com/2013/09/rising-seas/if-ice-melted-map

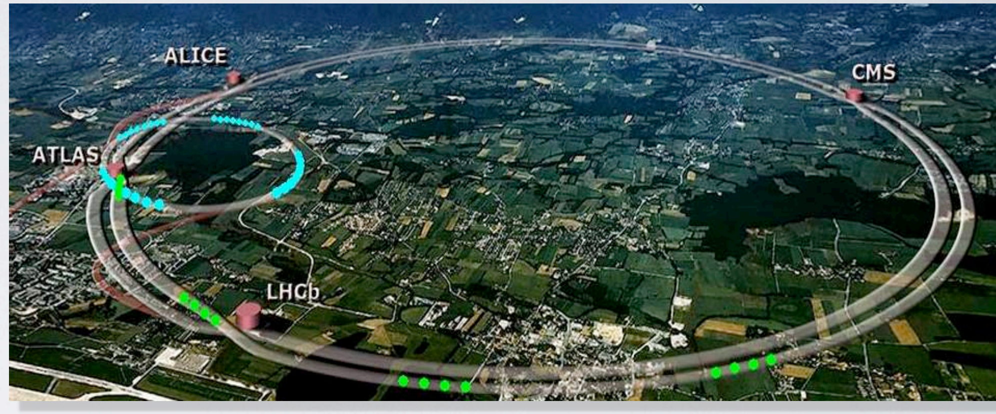
PART II

Mathematics and Computers to the Rescue

Experiments vs. Computational Science



75,000 increase



4.5 inches diameter

27 km circumference, $4B US

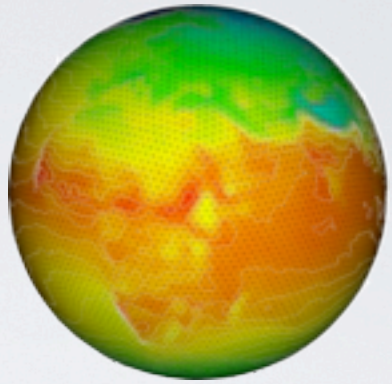
500 Million increase

400 operations/s, $500K

200 Billion operations/s, $400

Computational Science is now considered third pillar of science

Energy Efficiency
Tools for predicting building energy use



Earth Systems
Computer models for predicting extreme events

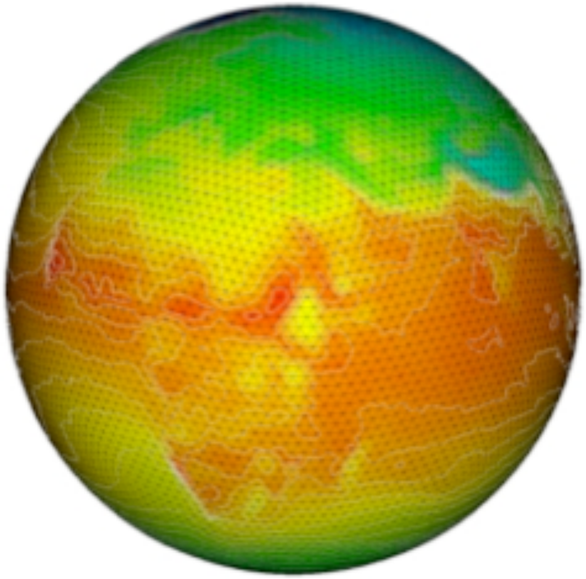
Energy Storage
Understanding and designing next-generation batteries

Combustion
Understanding the dispersion of pollutants in the environment.

Biofuels
Simulation models for understanding bottlenecks to economical biofuels

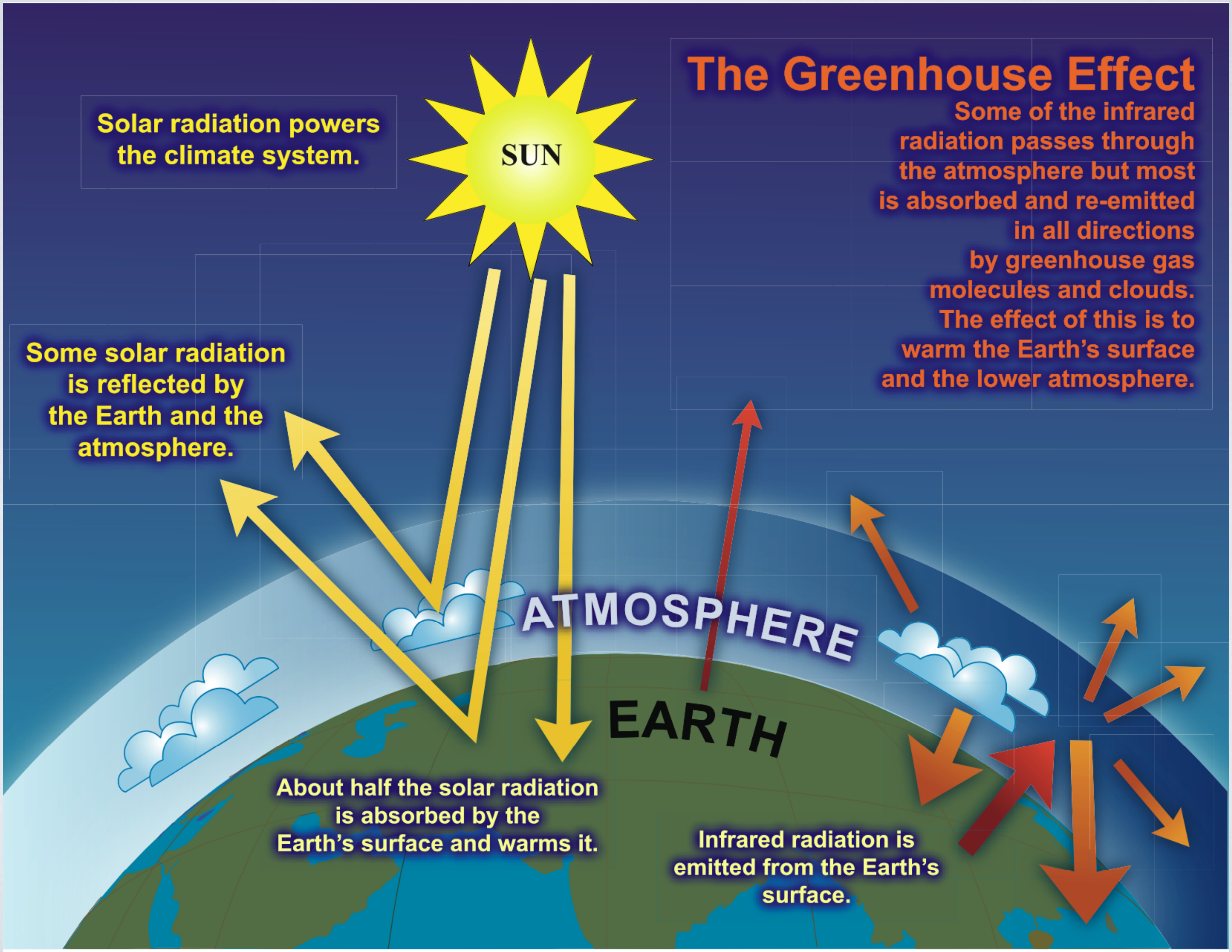
Nano Science
Predicting properties of next-generation photovoltaic solar cell materials.

Images courtesy of Lawrence Berkeley National Laboratory



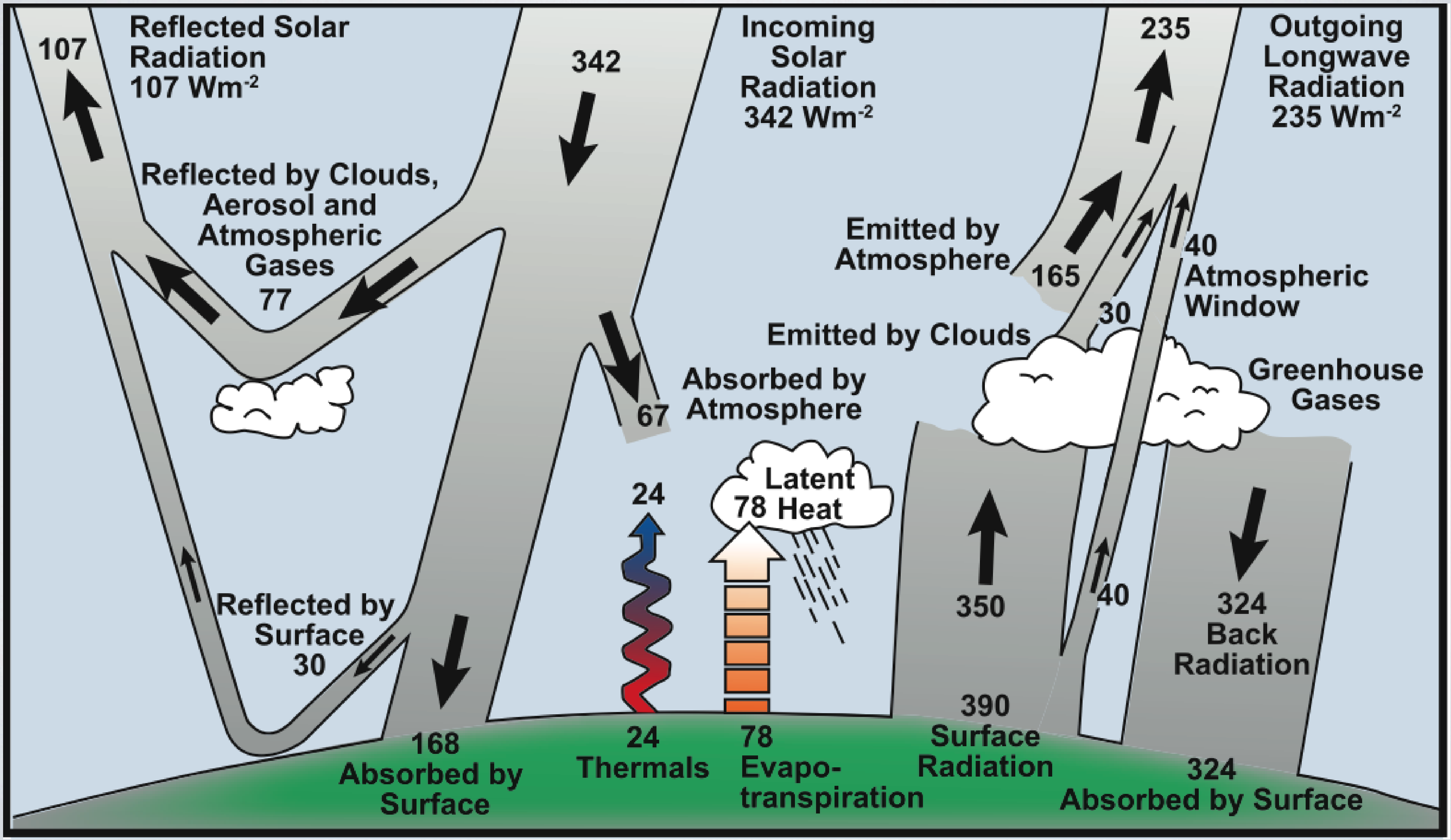
Climate Modeling

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

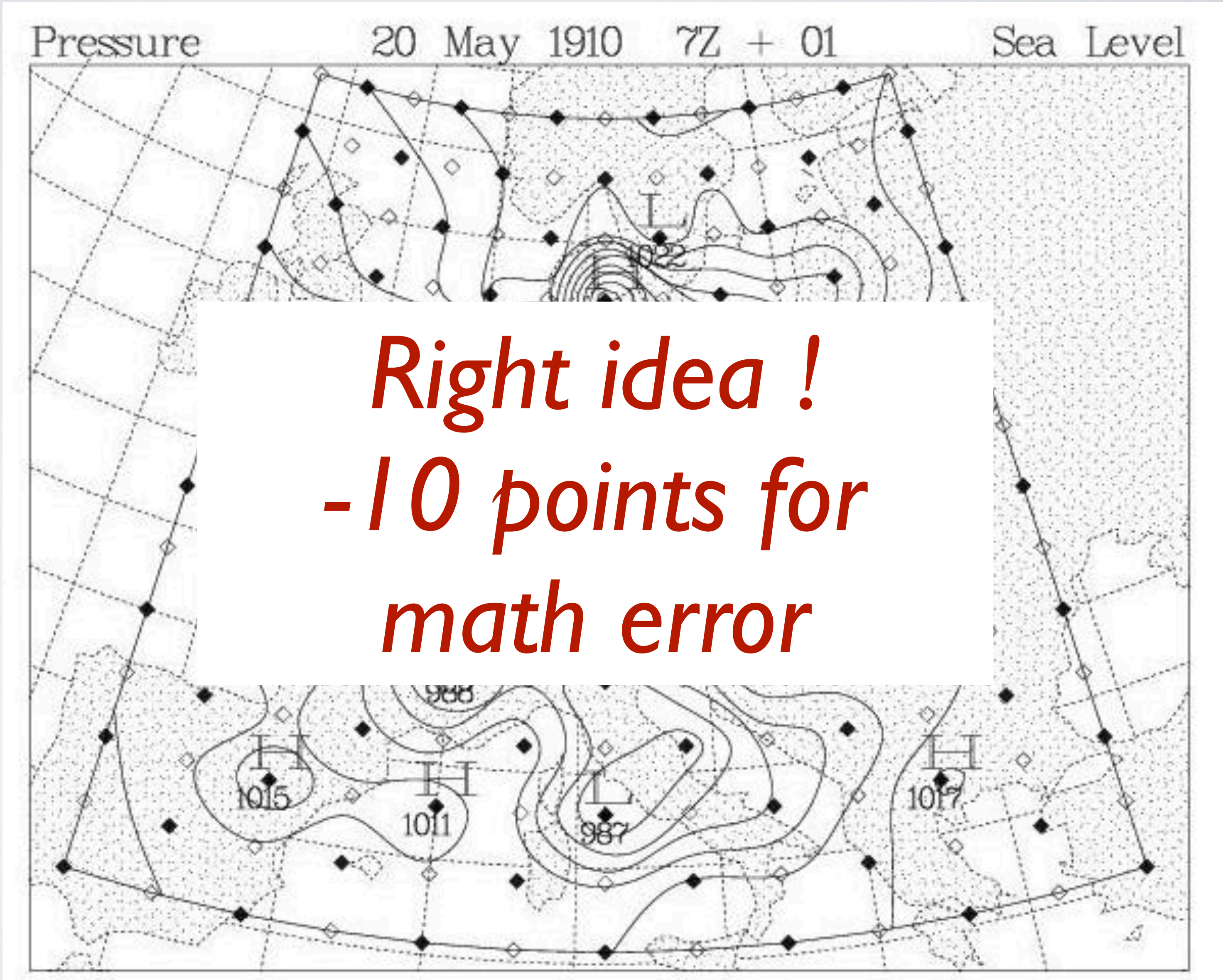
- British mathematician Lewis Fry Richardson proposed numerical weather forecasting in 1922
- Computed 1 day weather forecast over a period of 6 weeks,
- While working as the driver of a Quaker ambulance unit in northern France.

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

Sadly, calculations were unsuccessful, due to numerical problems



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

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

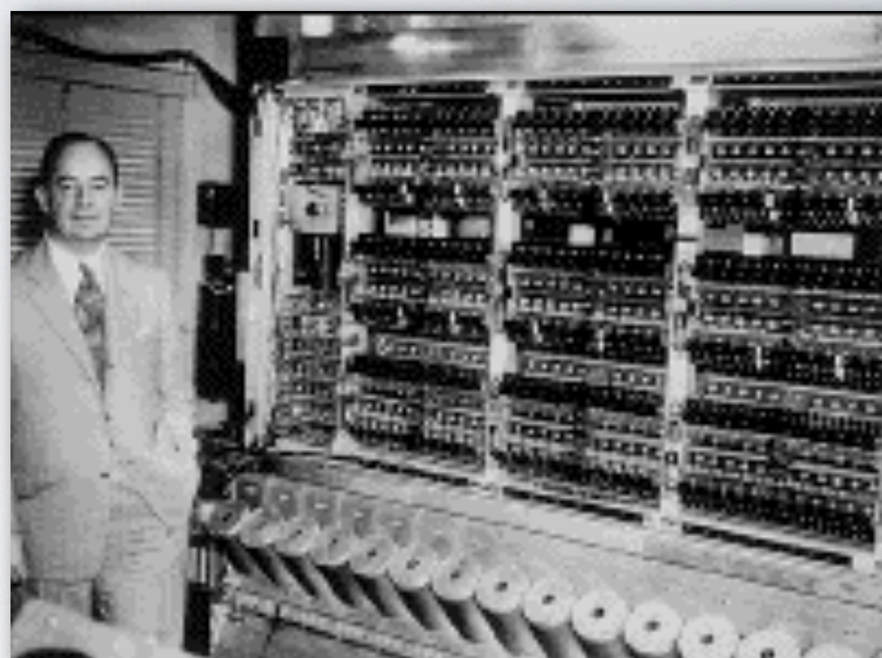
Conservation of energy

$$p = \rho RT$$

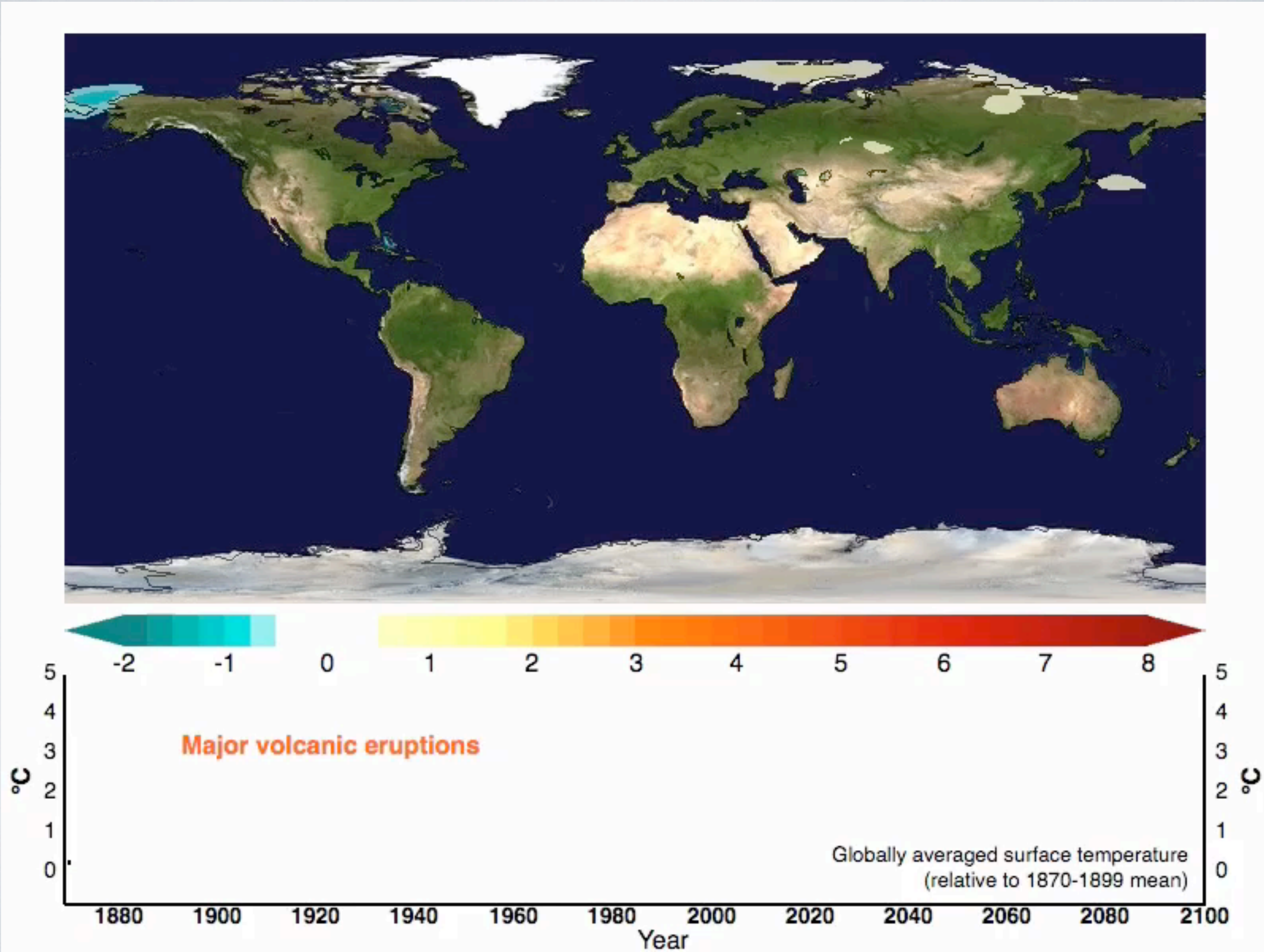
Equation of state

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

If burning fossil fuels is bad what are the alternatives?

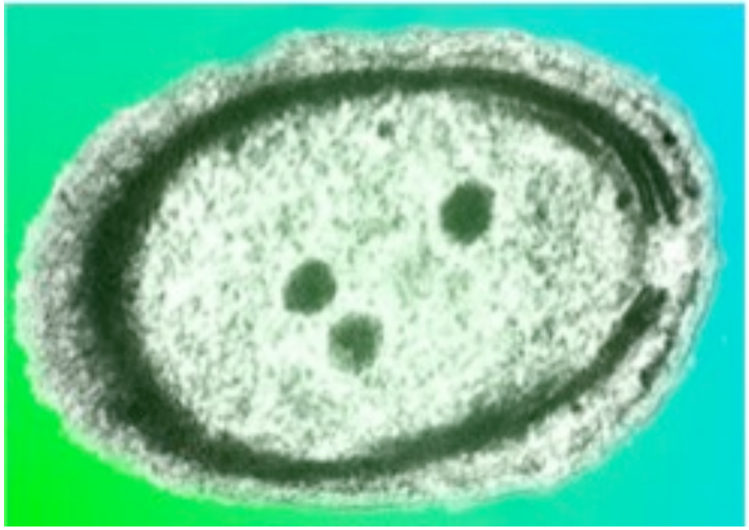
Solar Energy

Biofuels

Wind

Biofuels

PHOTOGRAPH COURTESY USDA-ARS VIA PNAS

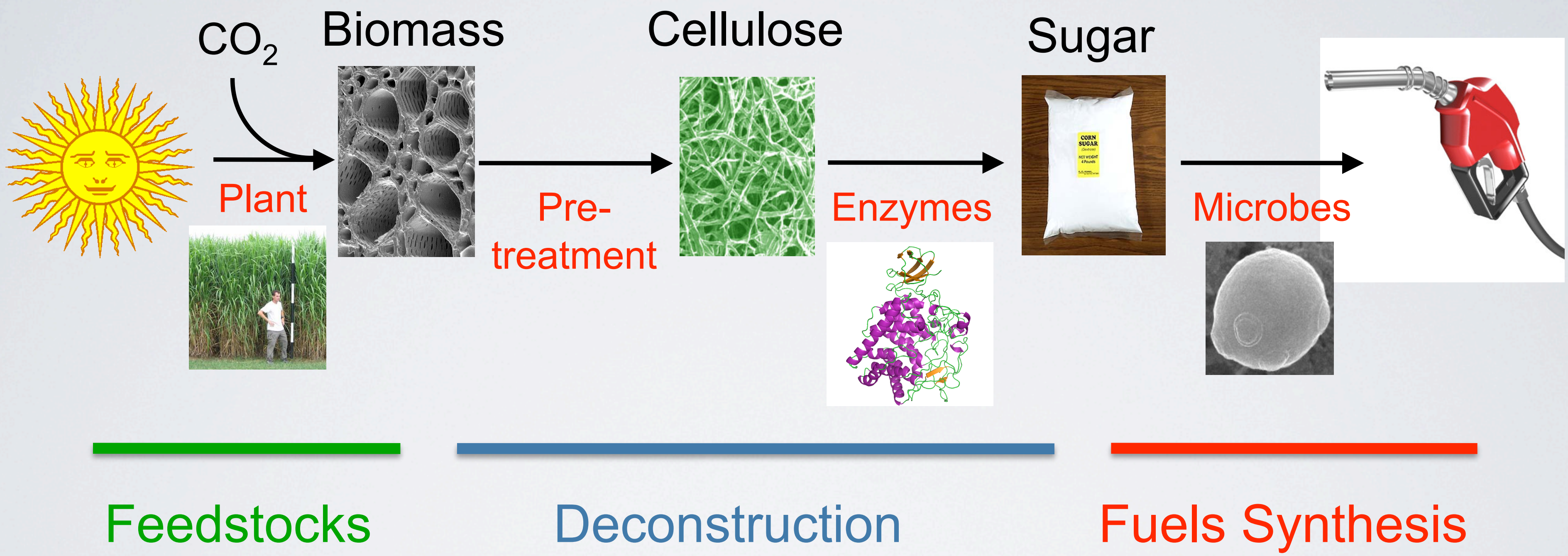


- Plants have evolved to be resistant to physical and chemical attack
- How do bacteria remove carbon from the atmosphere?
- If we can understand plant genomics better could we develop better biofuels?

RENEWABLE TRANSPORTATION FUELS

Perennial plants, such as switchgrass, provide an abundant source of power, generating five times as much energy as they take to grow

Biofuels - Cellulosic Transportation Fuels



Slide courtesy of P. Alivisatos, LBNL, Jan. 29, 2010

BIOFUELS NOW BECOMING ECONOMICALLY VIABLE

- Abengoa Bioenergy building a $500M plant to produce biofuels

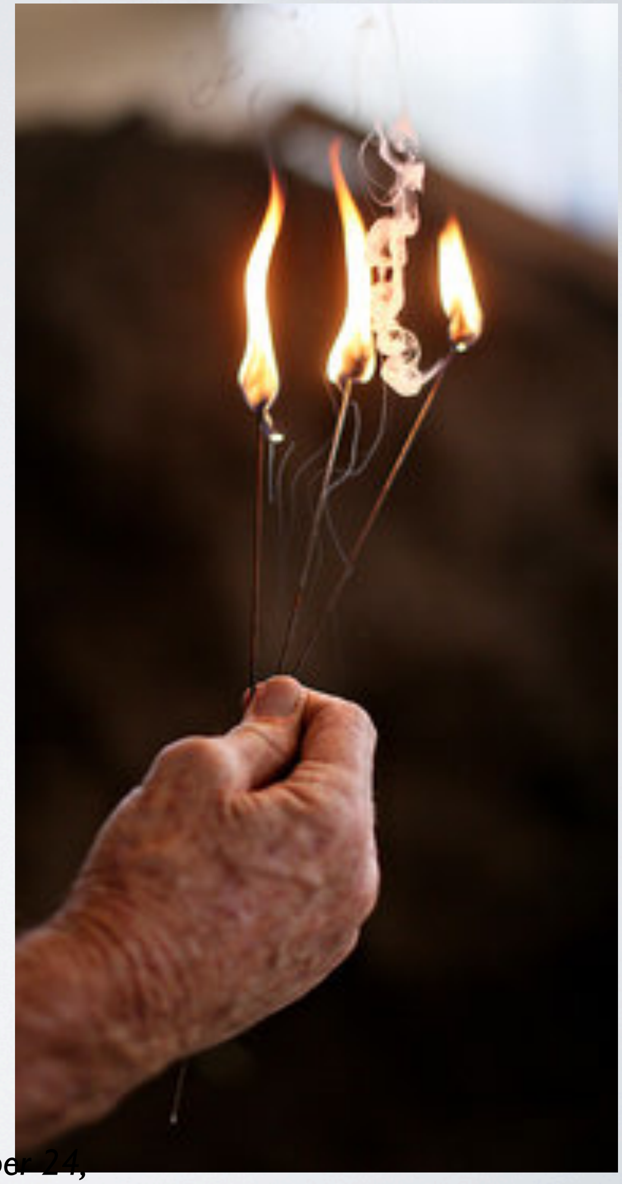
- Plans to produce 25M gallons of biofuels / year

- Based on cellulosic ethanol from corn stalks and wheat straw

http://www.nytimes.com/2014/04/15/business/energy-environment/dual-turning-point-for-biofuels.html?_r=0

PLANT SEEDS AS BIOFUELS

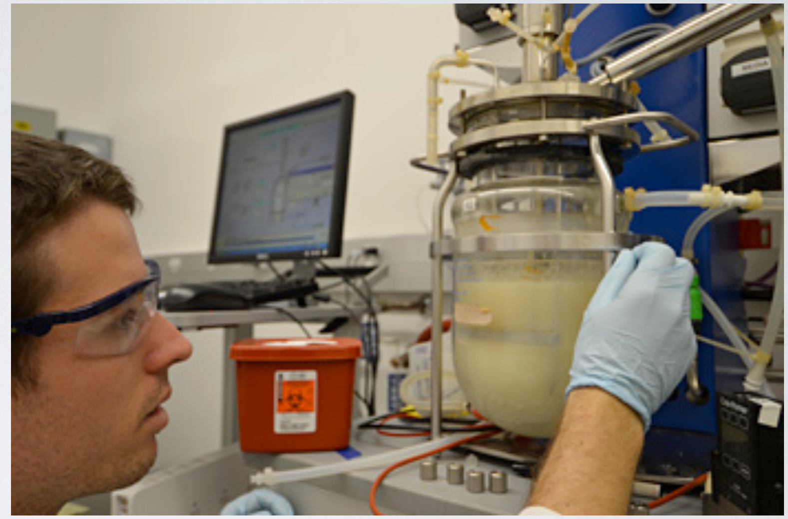
- Company plans to have 250,000 acres of jatropha in Brazil, India and other countries
- Expected to eventually produce about 70 million gallons of fuel a year.
- Advances in molecular genetics and DNA sequencing technology led to domesticating jatropha in a few years, a process that once took decades



Start-Up Uses Plant Seeds for a Biofuel, By TODD WOODY, New York Times, December 24,

SUGAR TO DIESEL

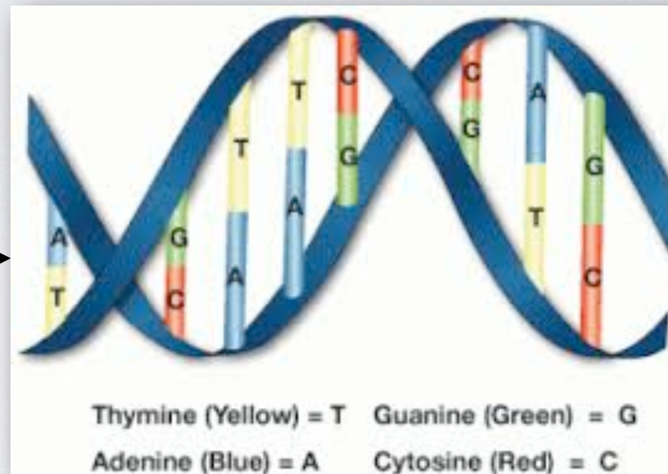
- UCB chemists and chemical engineers teamed up to produce diesel fuel from the products of a bacterial fermentation discovered nearly 100 years ago.
- The process produces a mix of products that contain more energy per gallon than ethanol
- Could be commercialized within 5-10 years



Graduate student Zachary Baer *works with a fermentation chamber in the Energy Biosciences Building to separate acetone and butanol (clear top layer) from the yellowish Clostridium brew at the bottom. Robert Sanders photo.*

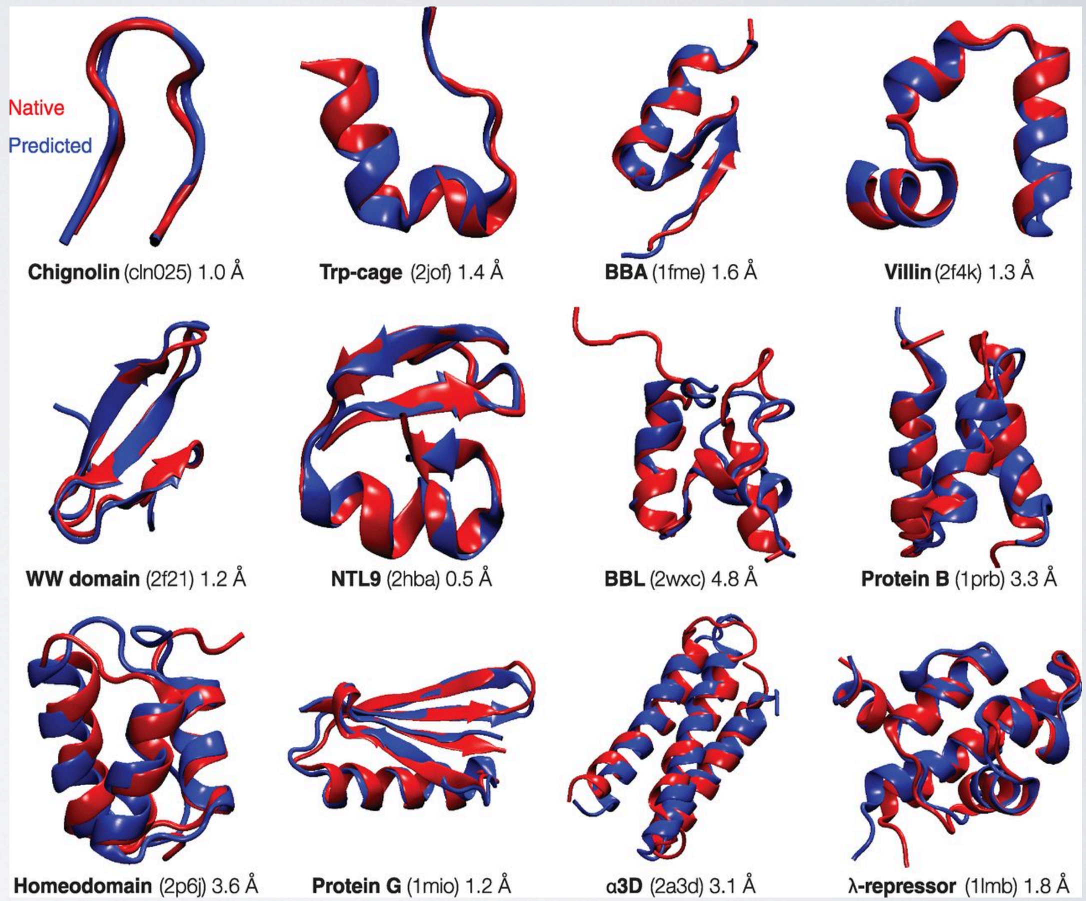
http://newscenter.berkeley.edu/2012/11/07/discovery-resurrects-process-to-convert-sugar-directly-to-diesel/
http://www.nature.com/nature/journal/v491/n7423/full/nature11594.html?WT.ec_id=NATURE-20121108

DNA TO PROTEINS



PROTEIN FOLDING PROBLEM

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

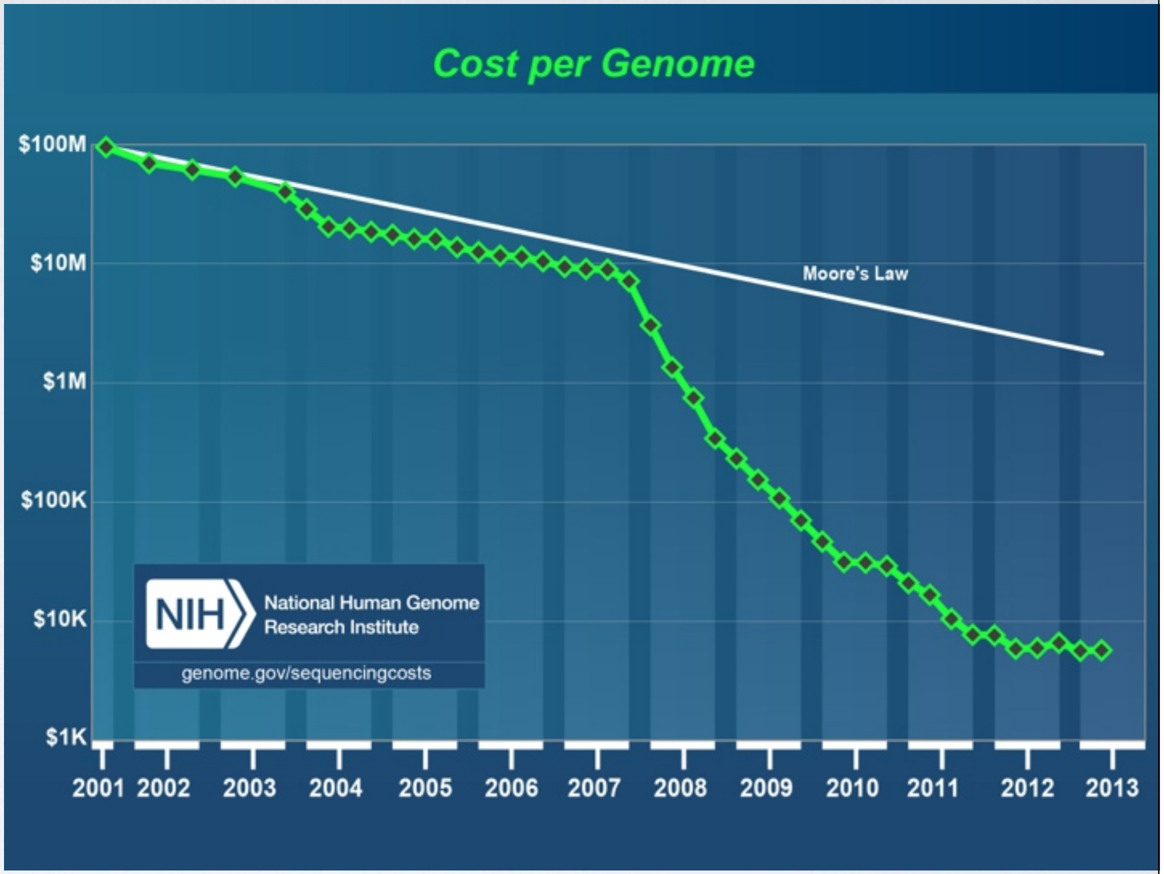


K A Dill, and J L MacCallum Science 2012;338:1042-1046

Science AAAS

DATA ENABLED SCIENCE

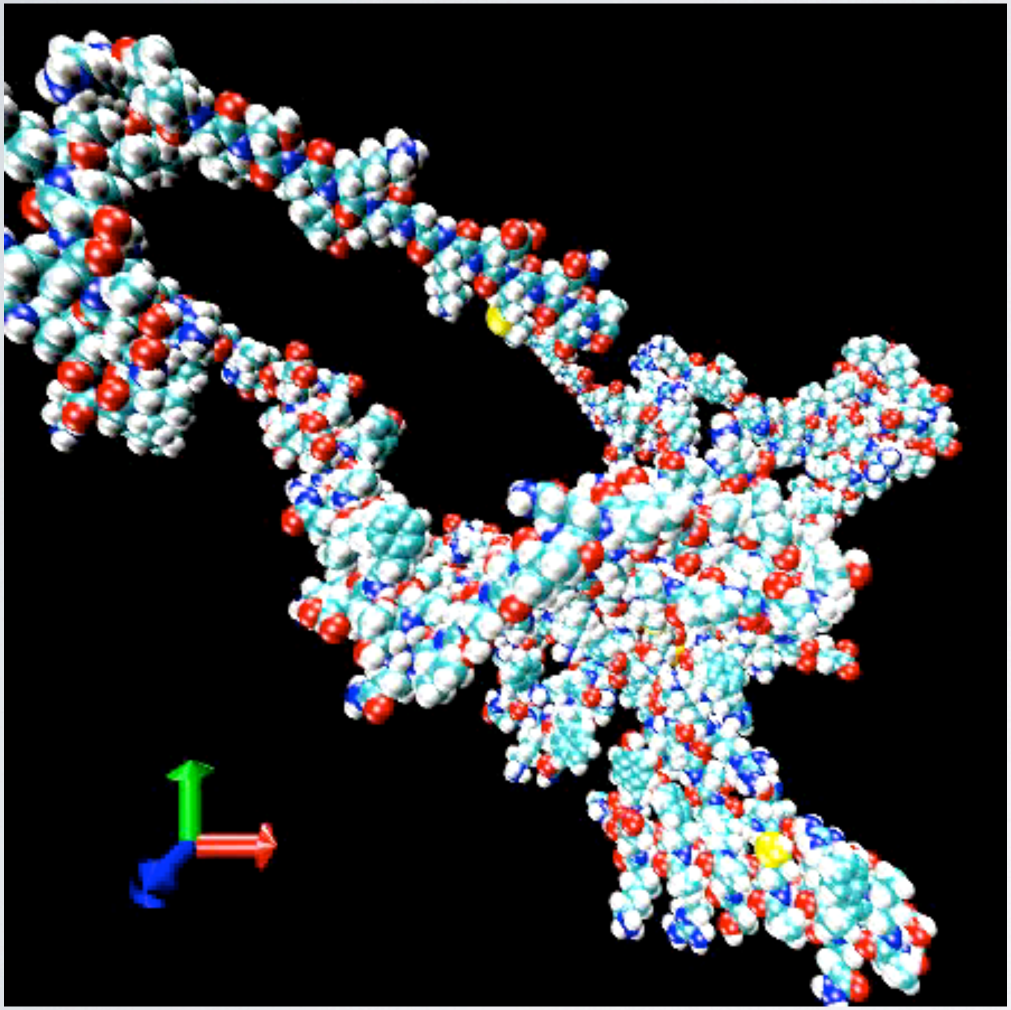
- Many scientific problems are now rate-limited by access to and analysis of data
- Genome sequencing is outpacing computing and algorithms
- High school students are now accessing and using genomic data for studies
- $1000 genome will soon be here



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

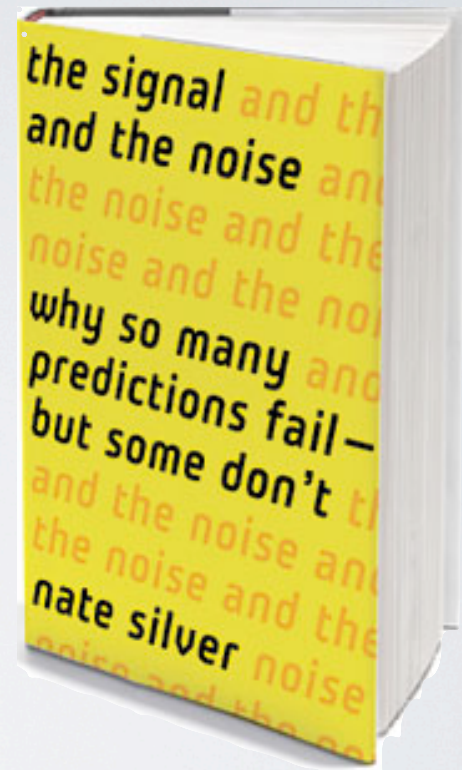


J.C. Meza et al. LBNL

- Computer (math) simulations can be used to predict 3D shapes of proteins
- Mathematical models can compute the energy of a molecule, which helps us understand their function
- Need new and better algorithms to analyze data

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



All models are wrong, but some models are useful. G.E.P. Box 1987

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?

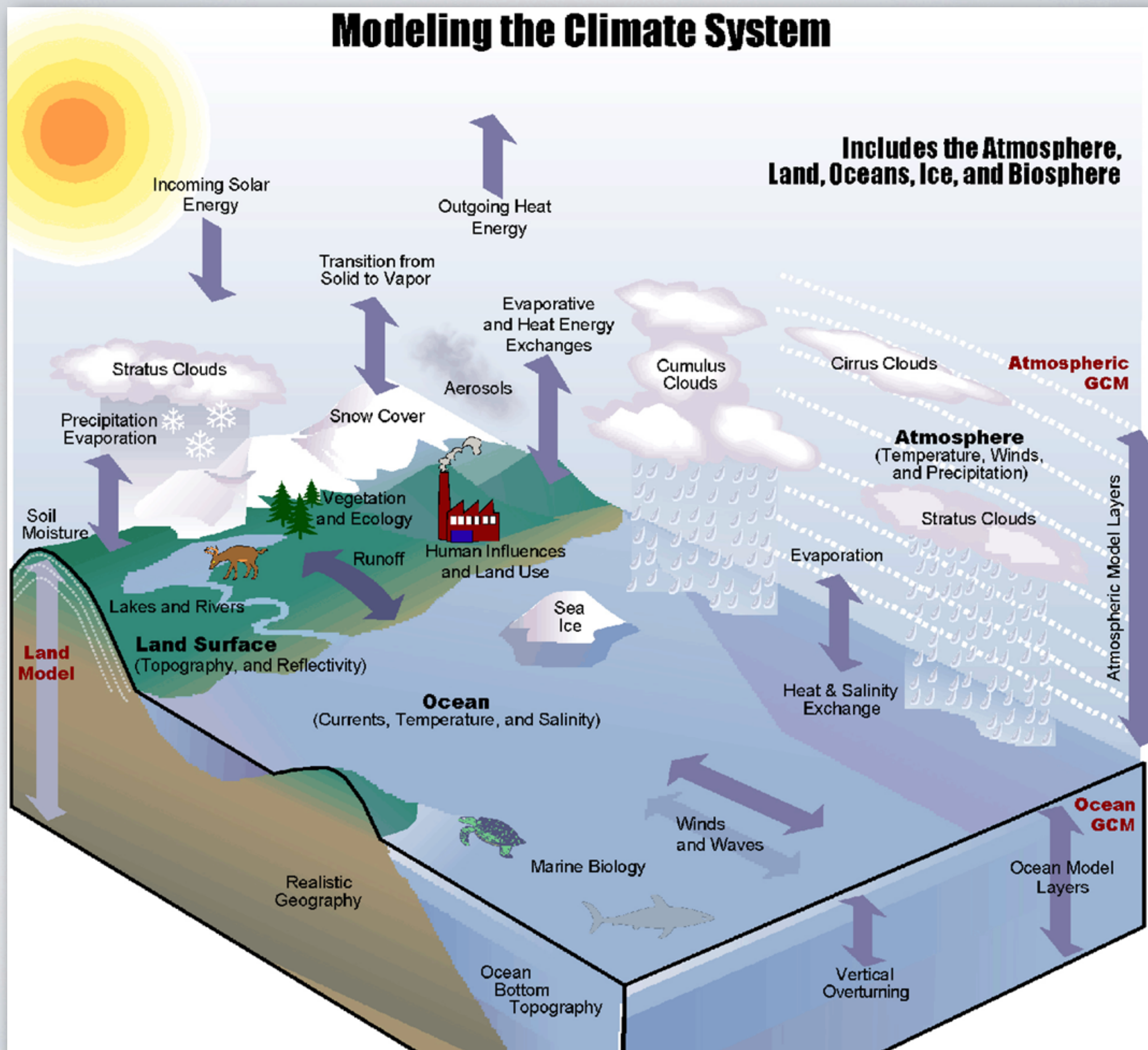
I'm Going To Help Save The World!


TRASH

SUPPLEMENTAL MATERIALS

CHALLENGES STILL EXIST FOR BIOFUELS

- Don't have the full fuel value of gasoline
- Require energy-intensive purification processes
- Toxic at high concentrations


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
Soil Moisture
Stratus Clouds
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

Fun Biofuel Facts

- Ethanol reduces greenhouse gas emissions up to 65 percent [source: Nebraska Ethanol Board].
- Perennial plants, such as switchgrass, provide an abundant source of power, generating five times as much energy as they take to grow [source: Biello].
- Biodiesel vehicles get 30 percent better fuel economy than gasoline-powered vehicles [source: Consumer Reports].