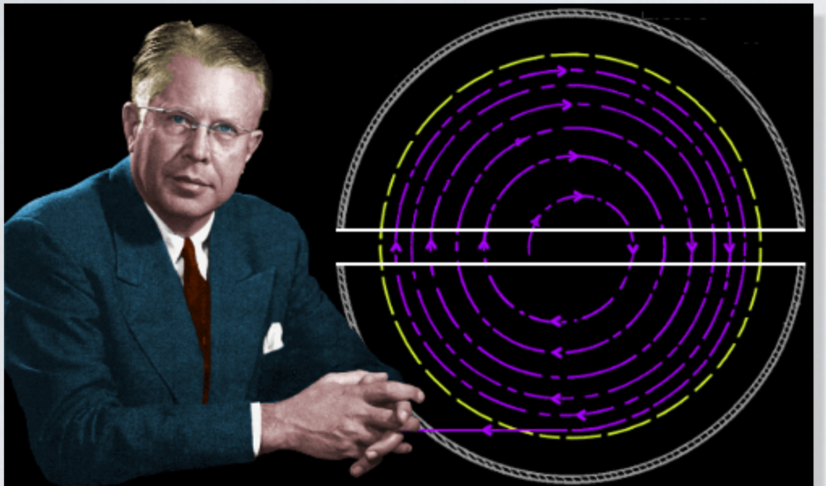
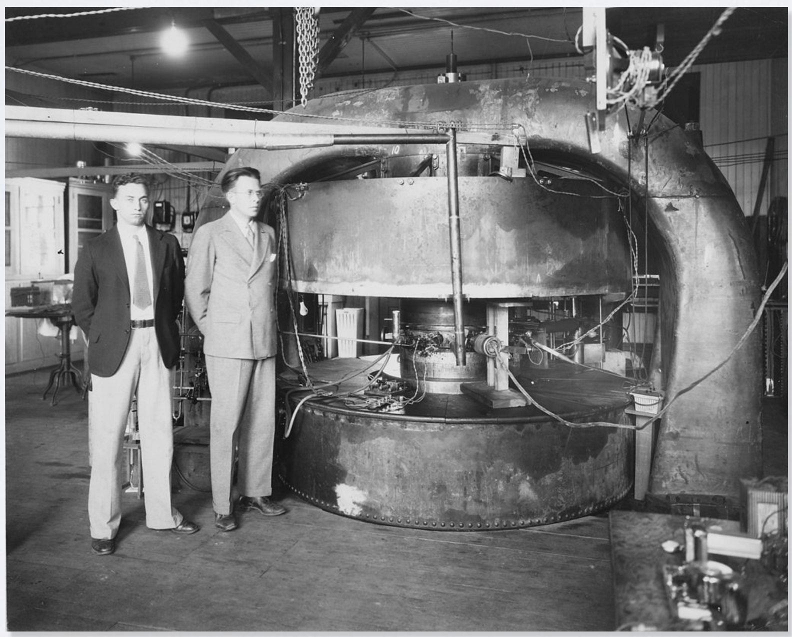
Computational Math and Science

How Mathematics Will Help Save The World

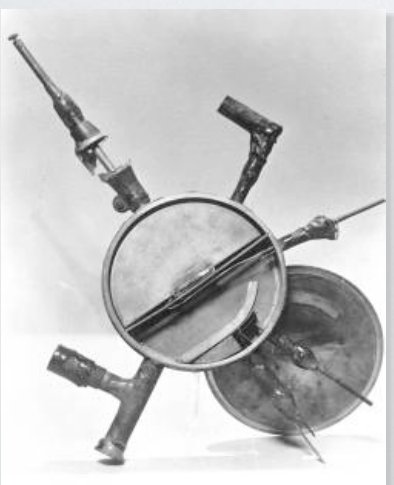
Juan Meza
Professor Applied Mathematics
Dean, School of Natural Sciences, UC Merced

Birth of Big Science





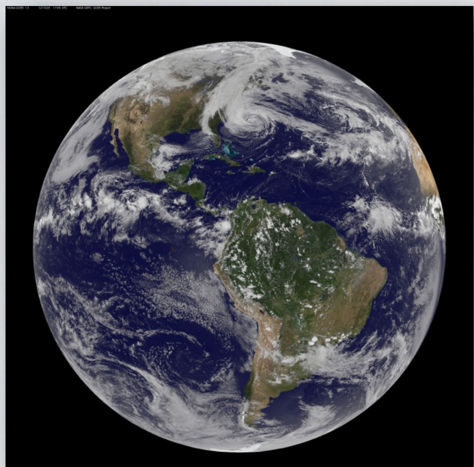
27 km
circumference
7 TeV
$4B US
(2015)



27 inch (1934)

4.5 inches diameter, 80 keV (1931)

Let's do an experiment



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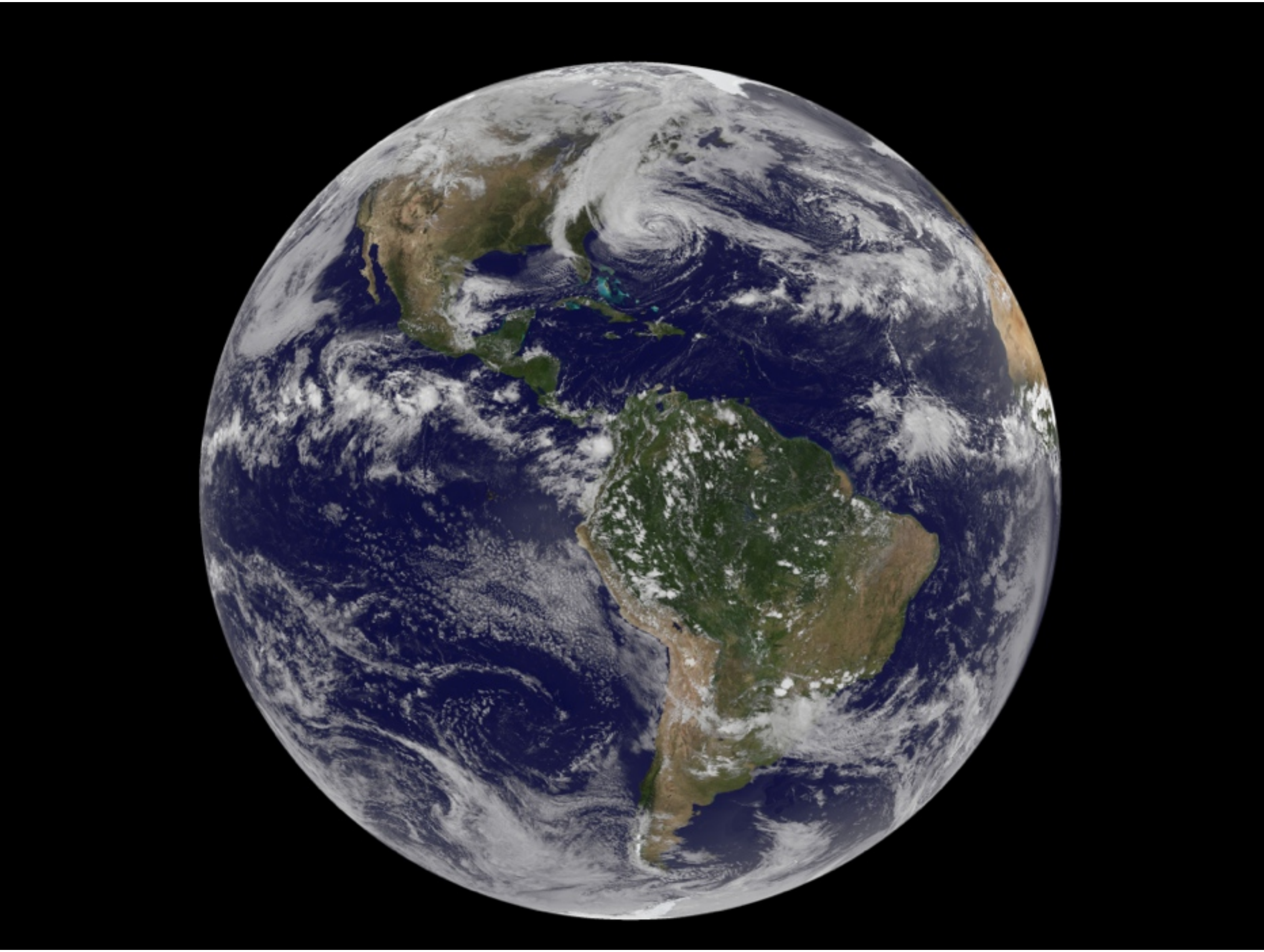
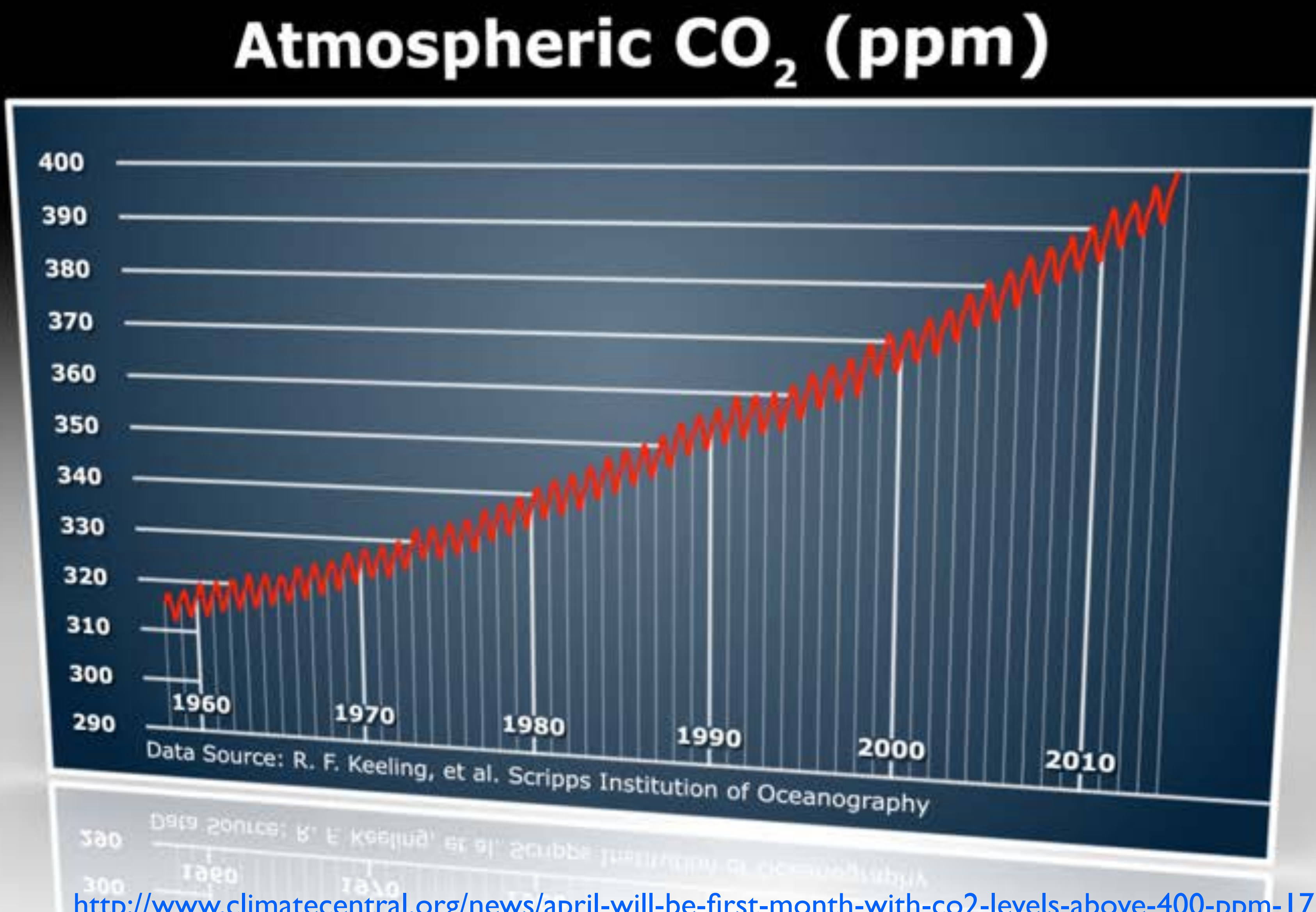
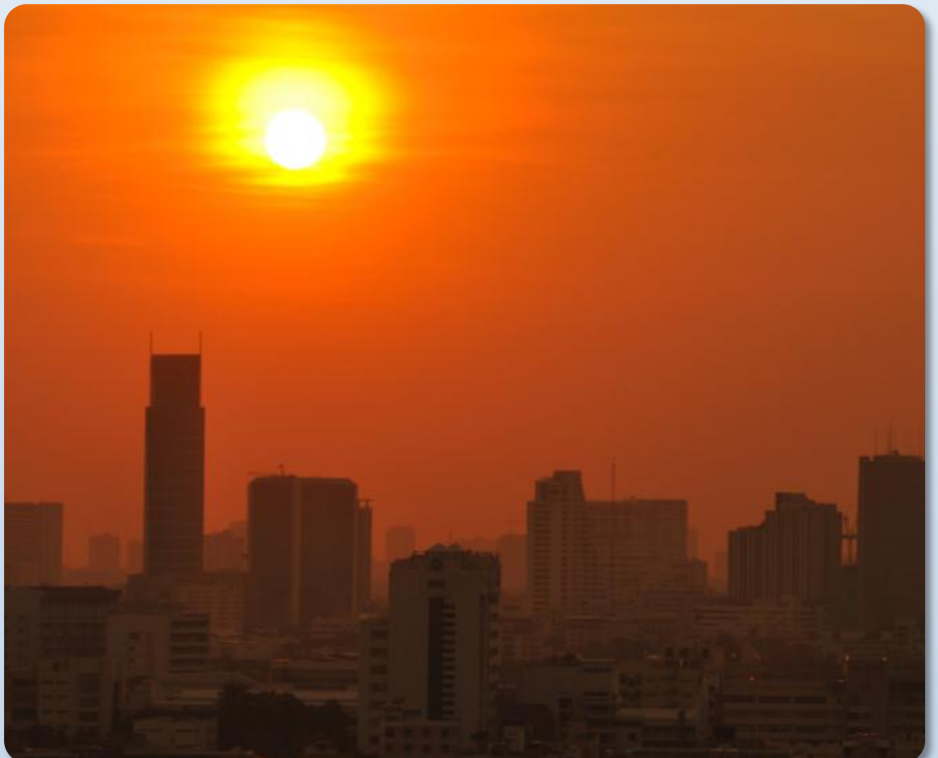


April 2014 Was The First Month With CO_2 Levels Above 400 PPM

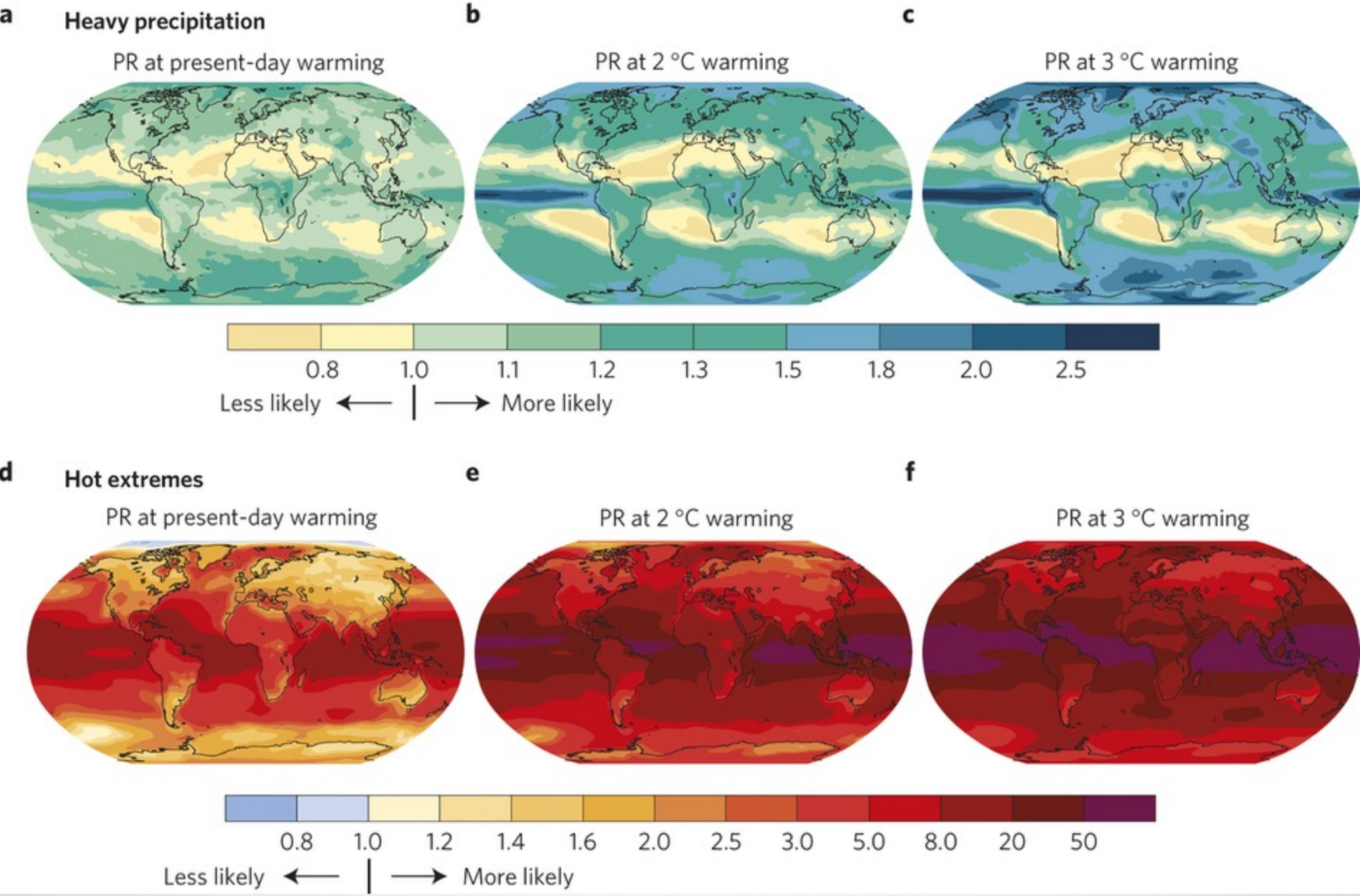


http://www.climatecentral.org/news/april-will-be-first-month-with-co2-levels-above-400-ppm-17331

Since 1950, extreme hot days and heavy precipitation have become more common



There is evidence that anthropogenic influences, including increasing atmospheric greenhouse gas concentrations, have changed these extremes

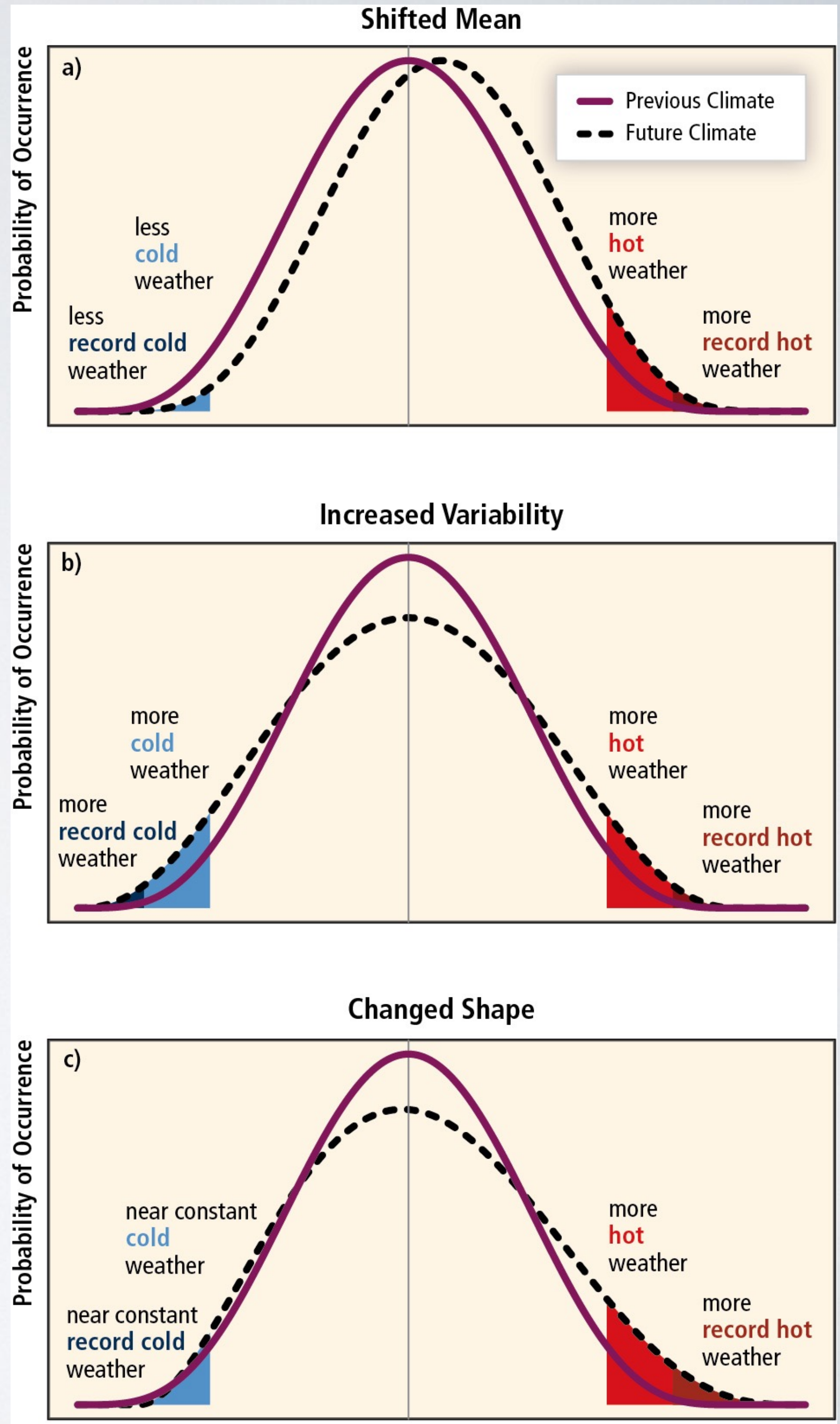


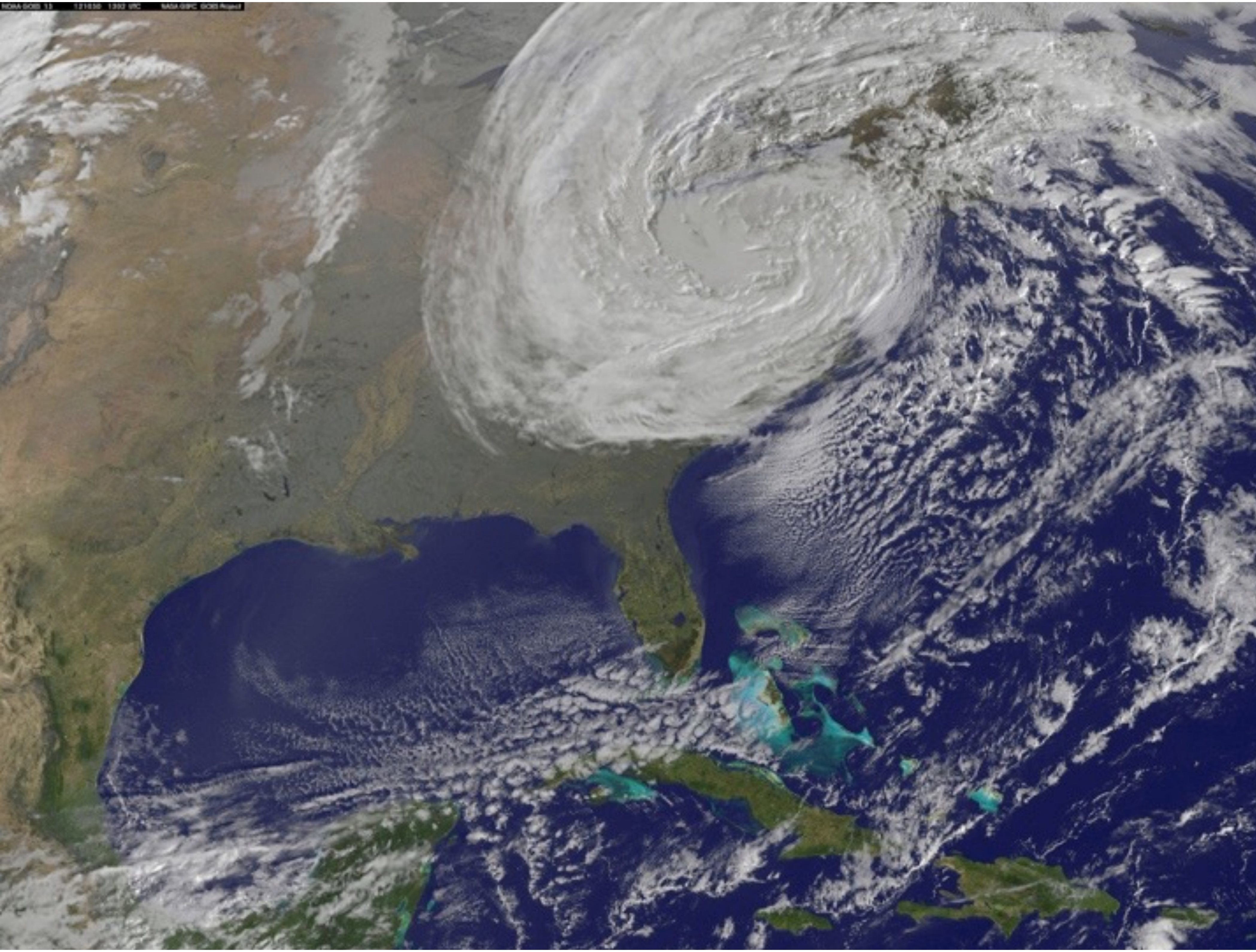
E. M. Fischer* and R. Knutti, Nature Climate Change, 27 April 2015, DOE:10.1038/nclimate2617

- Changing climate leads to changes in extreme weather and climate events

- Extreme events affect agriculture, water, public health, transportation, etc.

- Economic losses can be enormous



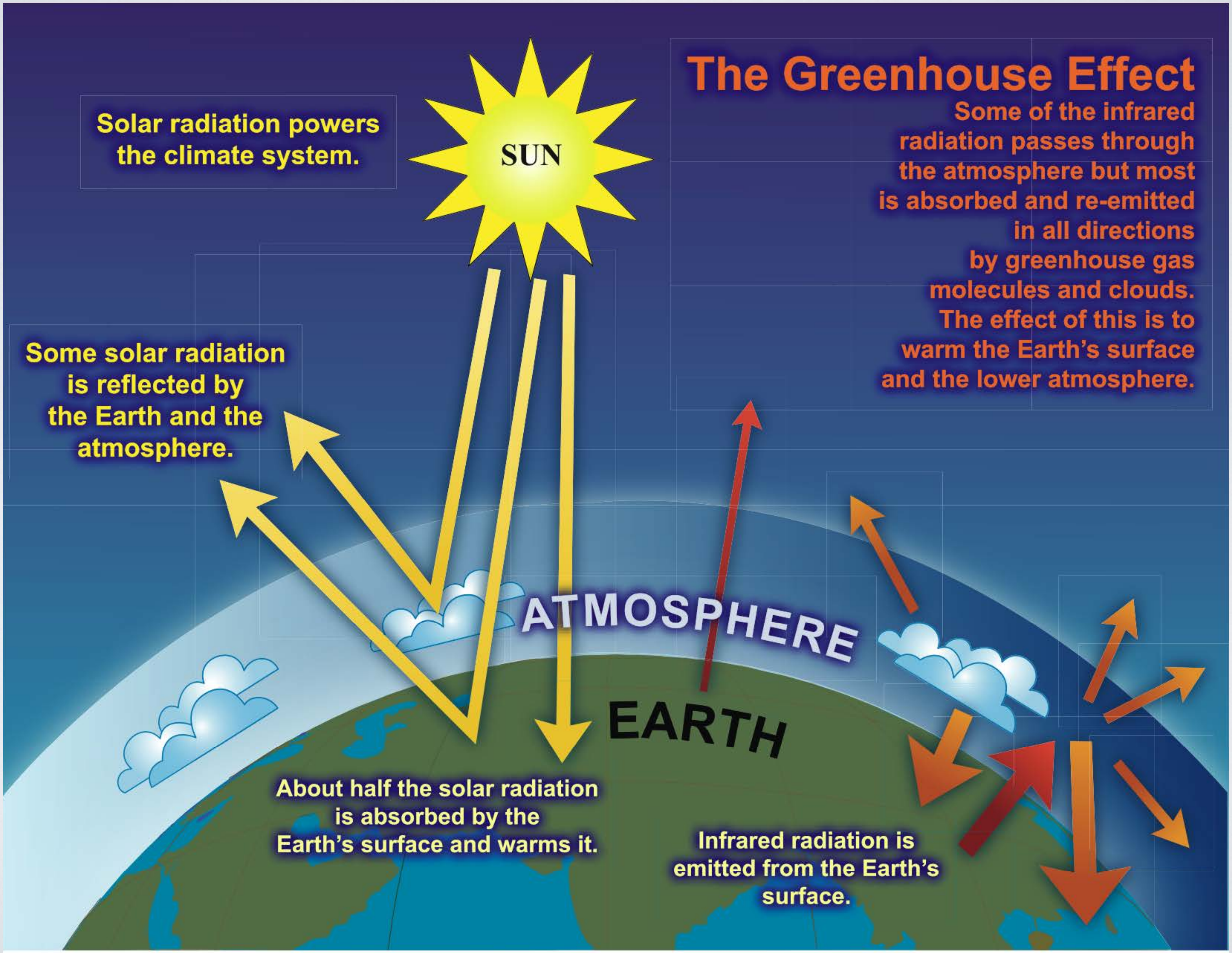

NOAA-GOES 13
NASA-GSFC GOES Project

PART II

Mathematics and Computers to the Rescue

First Let's Look at the Mathematics

GREENHOUSE EFFECT



FIRST MENTION OF GREENHOUSE EFFECT (1824)

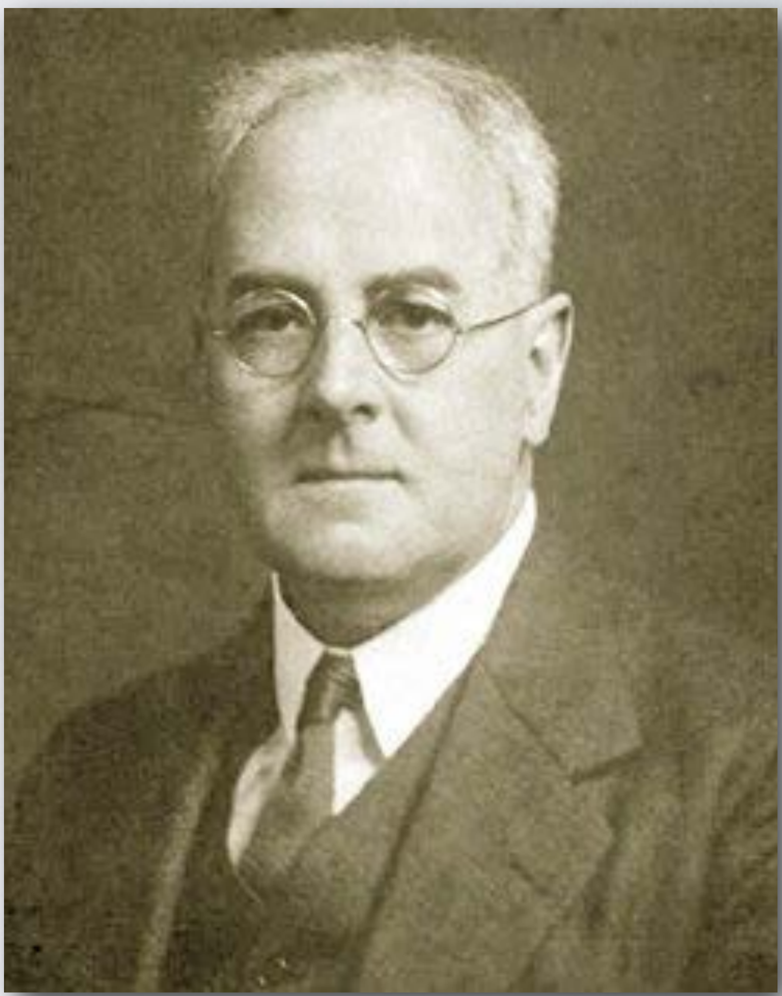
- Fourier developed mathematical theory for the temperature of the terrestrial globe

- "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.

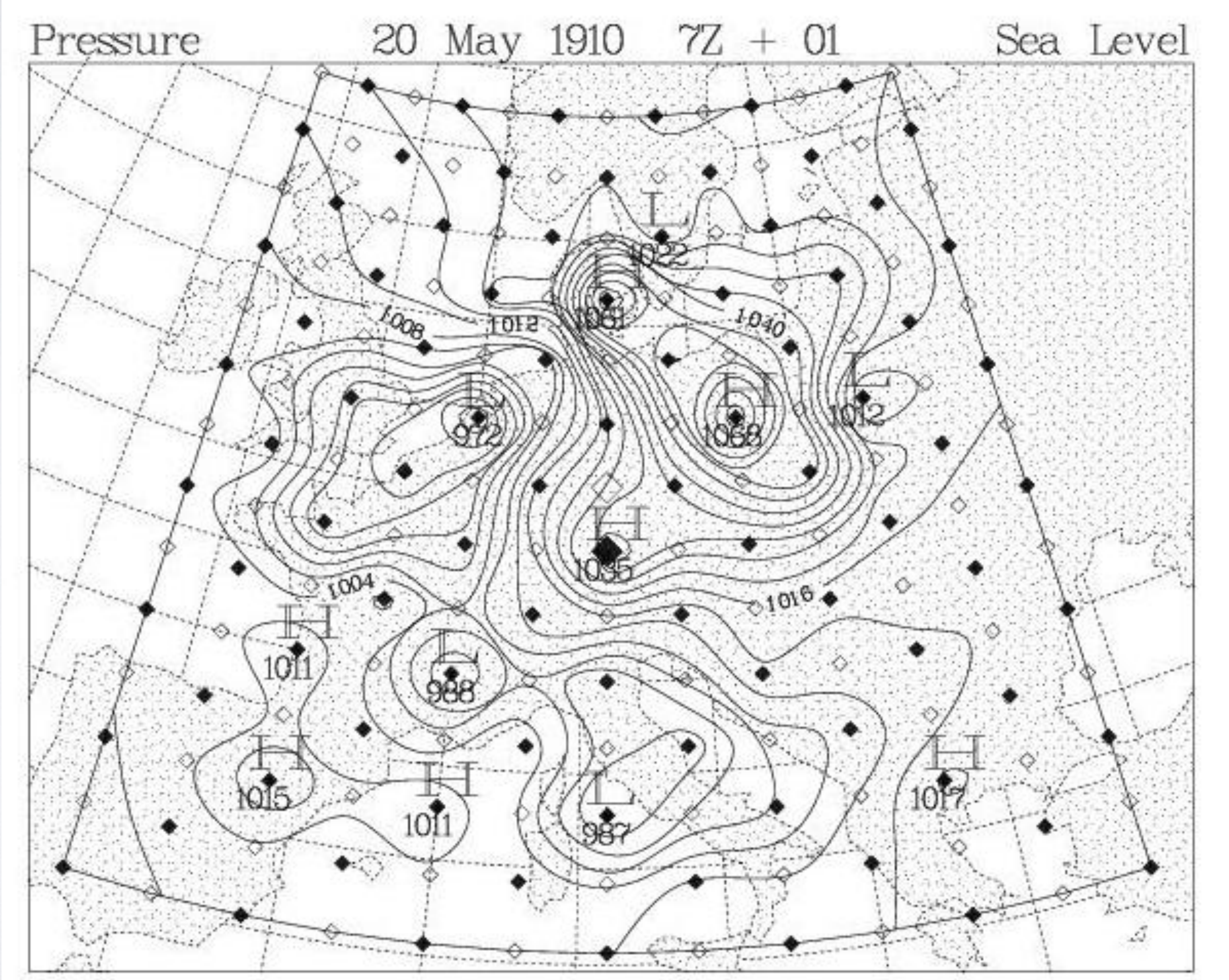


LEWIS FRY RICHARDSON

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

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

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

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

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

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

$$p = \rho RT$$

PRIMITIVE EQUATIONS FOR ATMOSPHERE

Conservation of momentum

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

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

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

Conservation of mass

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

Conservation of energy

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

Equation of state

$$p = \rho R T$$

Where do Computers Fit In To the Picture?

Babbage's Difference Engine (1832)

"As soon as an Analytical Engine exists, it will necessarily guide the future course of the science."

http://www.computerhistory.org/babbage/engines/

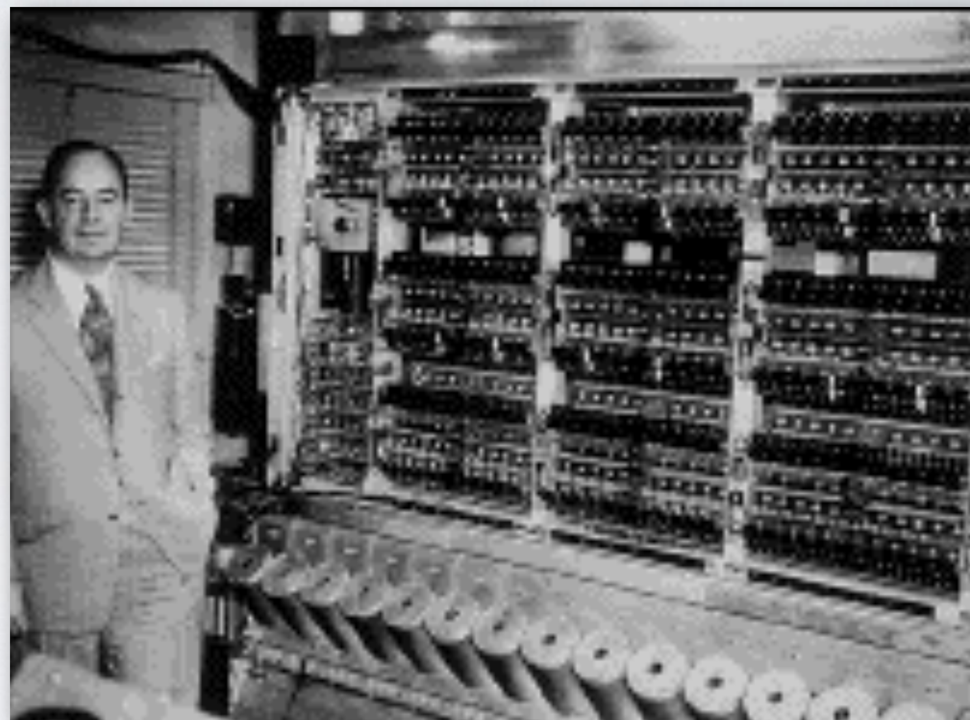
First Computer Programmer

- Described an algorithm for computing Bernoulli numbers on Babbage's Analytical Engine
- Suggested that computers could be used for purposes other than numbers
- Also pointed out a computer "bug" in Babbage's equations

Ada Lovelace

JOHN VON NEUMANN'S METEOROLOGY PROJECT

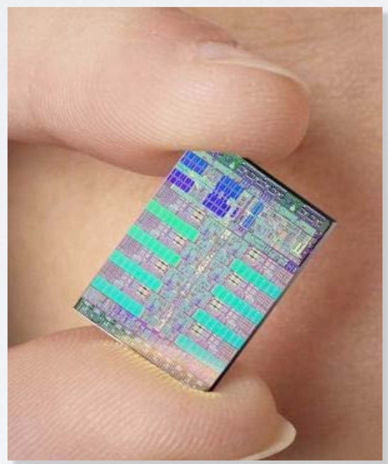
- Recognized numerical weather forecasting as a problem of great importance
- In collaboration with Charney and Fjortoft, they completed the first numerical computer forecast in 1950
- Used ENIAC, first multipurpose electronic digital computer
- Each 24 hour forecast took 24 hours to compute



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

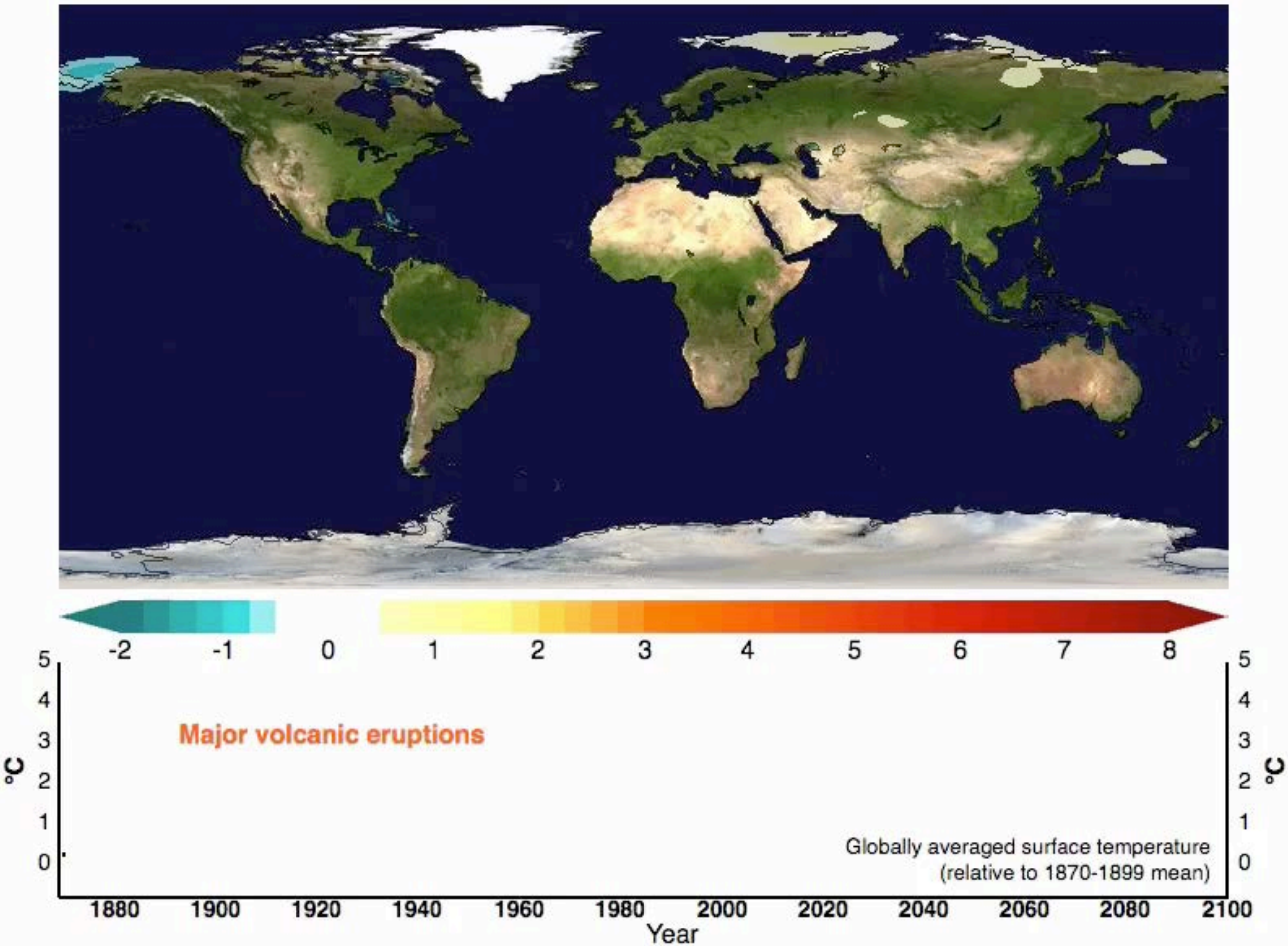
93,000,000,000,000,000

33.8 TFlops/s (2014)
93,000 TFlops/s (2016)



200 Billion operations/s
$400 (2005)

400 operations/s, $500K (1946)


-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

PRECAUTIONARY PRINCIPLE

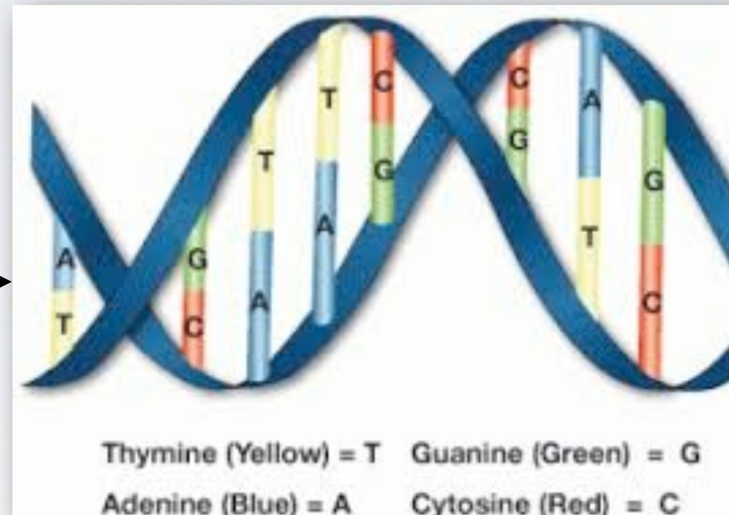
"When an activity raises threat of harm to human health or the environment, precautionary measures should be taken even if some cause and effect relationships are not fully established scientifically. In this context, the proponent of an activity, rather than the public, should bear the burden of proof."

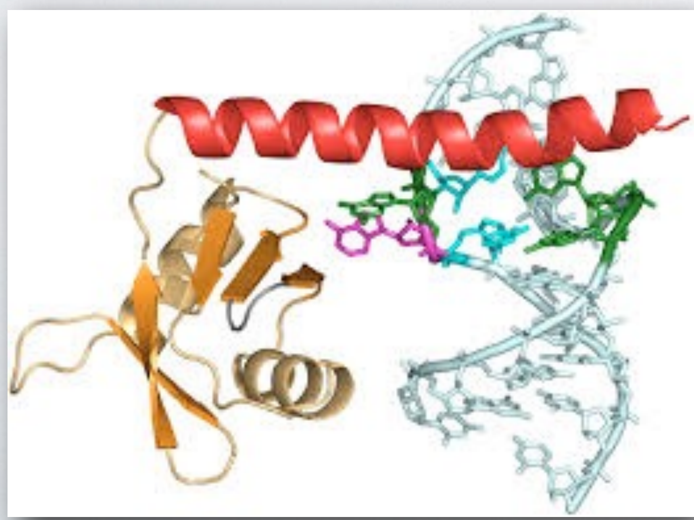
Sandra Steingraber, Living Downstream, pp. 290

PART III

Connections To Living Downstream

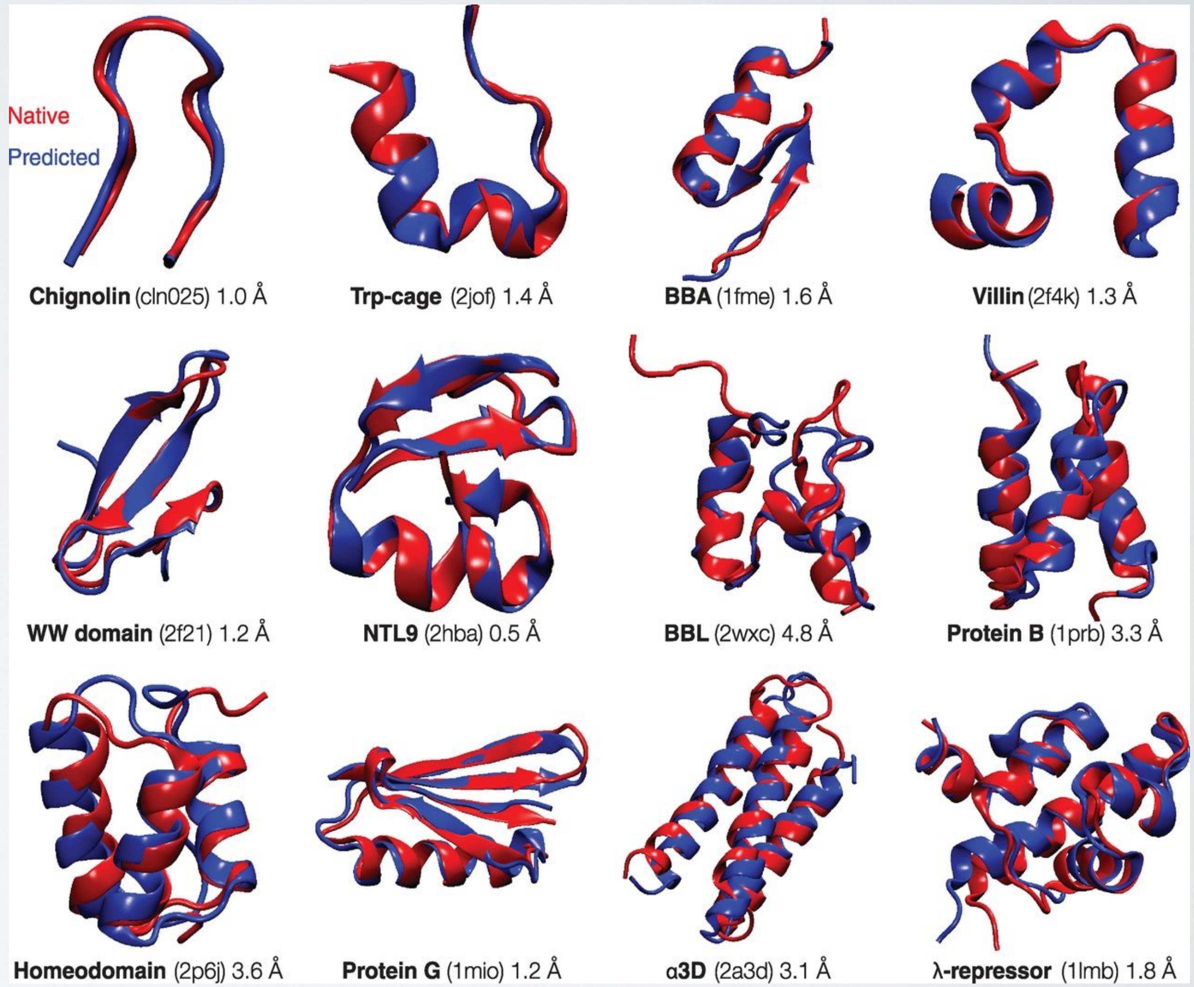
UNDERSTANDING CANCER: DNA TO PROTEINS





PROTEIN FOLDING PROBLEM

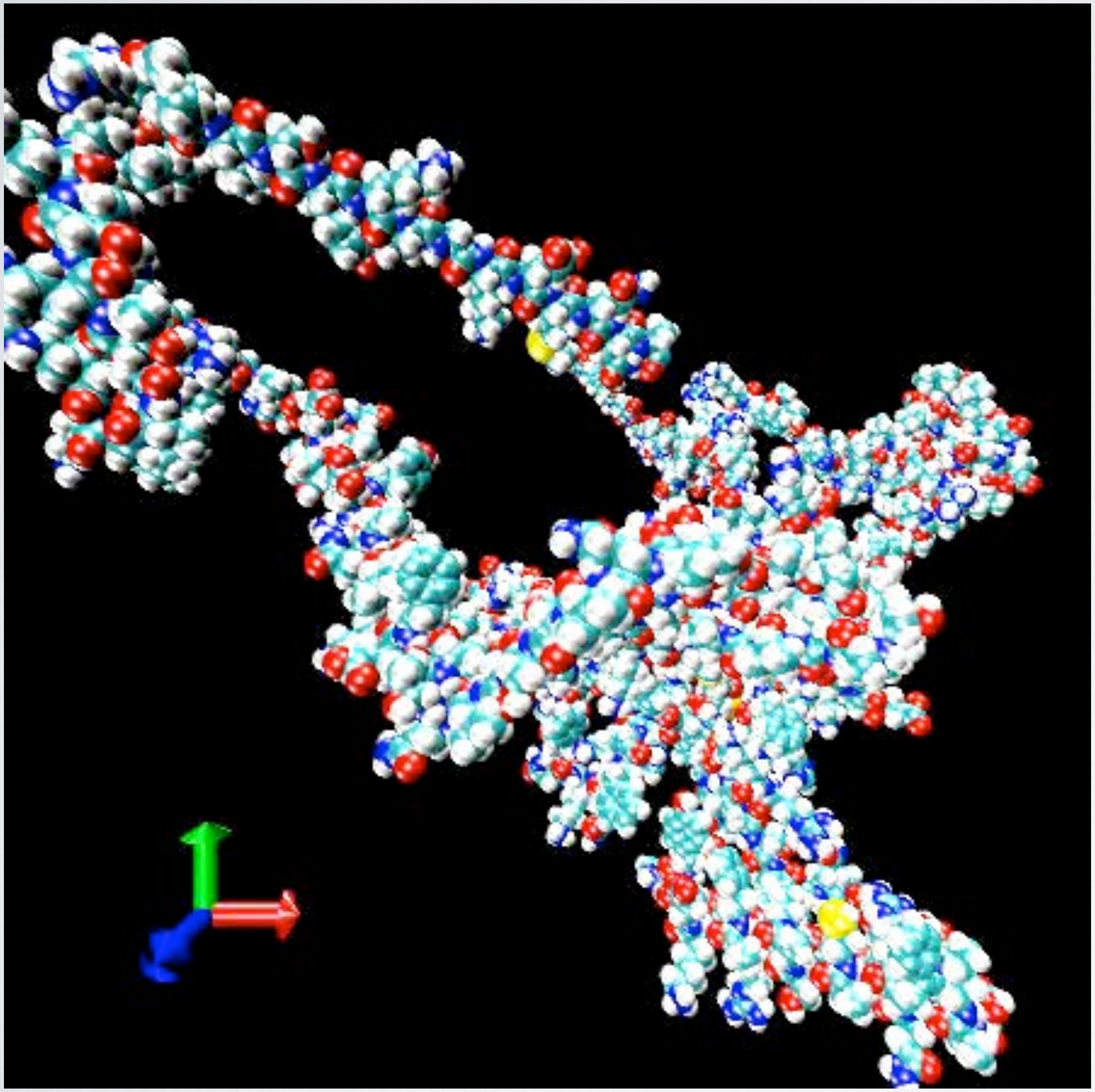
- Genome sequence is only the start
- The 3D shape of a protein determines its function
- One of the grand scientific challenges



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

Science
AAAS

PROTEIN FOLDING

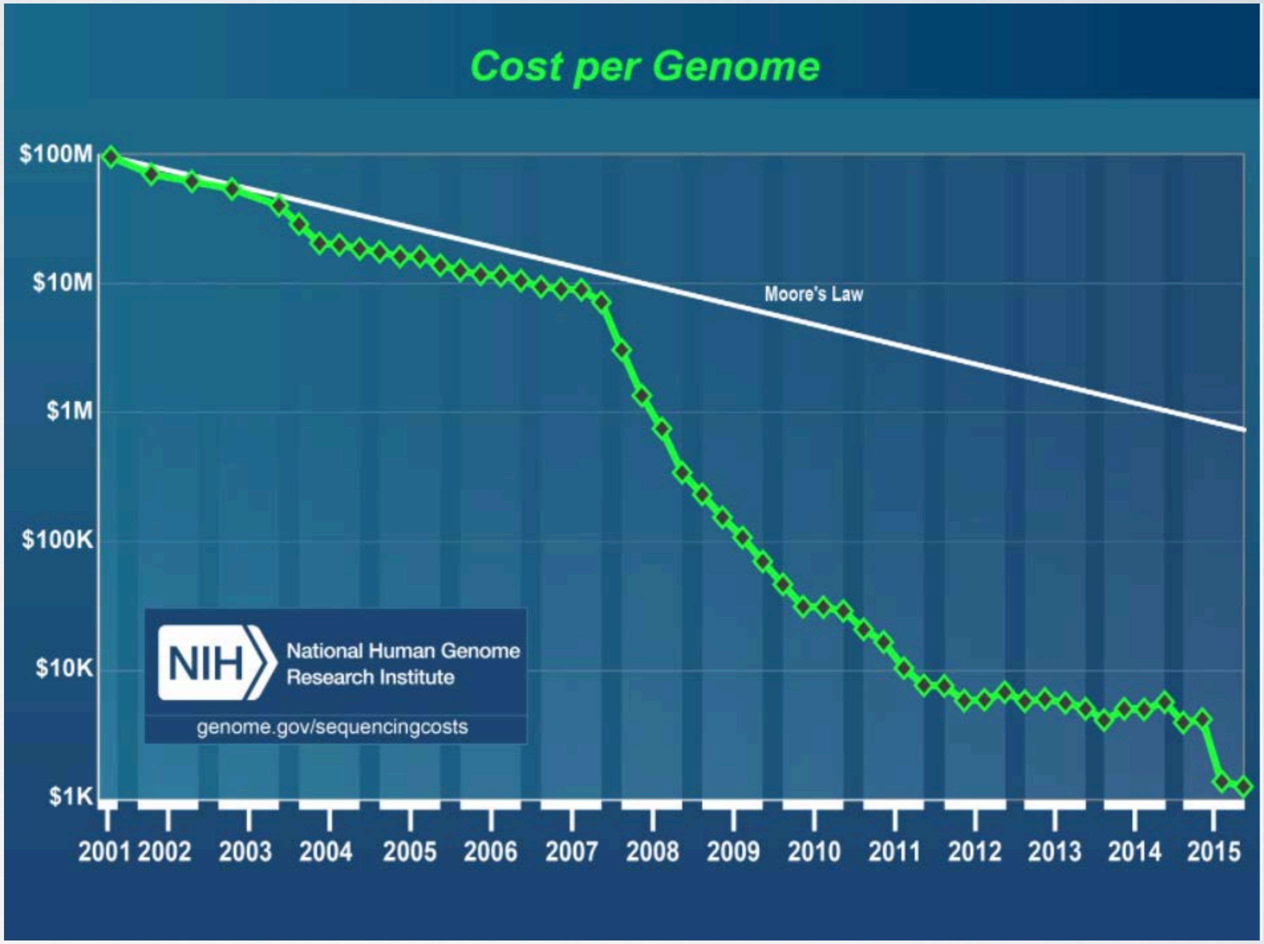


J.C. Meza et al. LBNL

- 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

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



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)

November 30, 2011

DNA Sequencing Caught in Deluge of Data

By ANDREW POLLACK

BGI, based in China, is the world's largest genomics research institute, with 167 DNA sequencers producing the equivalent of 2,000 human genomes a day.

BGI churns out so much data that it often cannot transmit its results to clients or collaborators over the Internet or other communications lines because that would take weeks. Instead, it sends computer disks containing the data, via FedEx.

WIRED MAGAZINE: 16.07

SCIENCE : DISCOVERIES

The End of Theory: The Data Deluge Makes the Scientific Method Obsolete

By Chris Anderson 06.23.08

Illustration: Marian Bantjes

THE PETABYTE AGE:
Sensors everywhere. Infinite storage. Clouds of processors. Our ability to capture, warehouse, and understand massive amounts of data is changing science, medicine, business, and technology. As our collection of facts and figures grows, so will

"All models are wrong, but some are use

So proclaimed statistician George Box 30 y he was right. But what choice did we have? from cosmological equations to theories of behavior, seemed to be able to consistently, imperfectly explain the world around us. I

the Atlantic

Print | Close

JOIN THE ATLANTIC ON FACEBOOK!

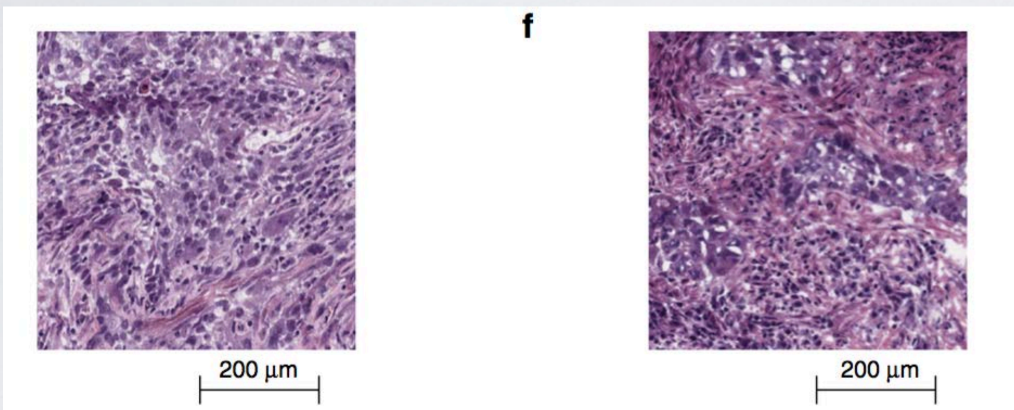
To Know, but Not Understand: David Weinberger on Science and Big Data

By David Weinberger

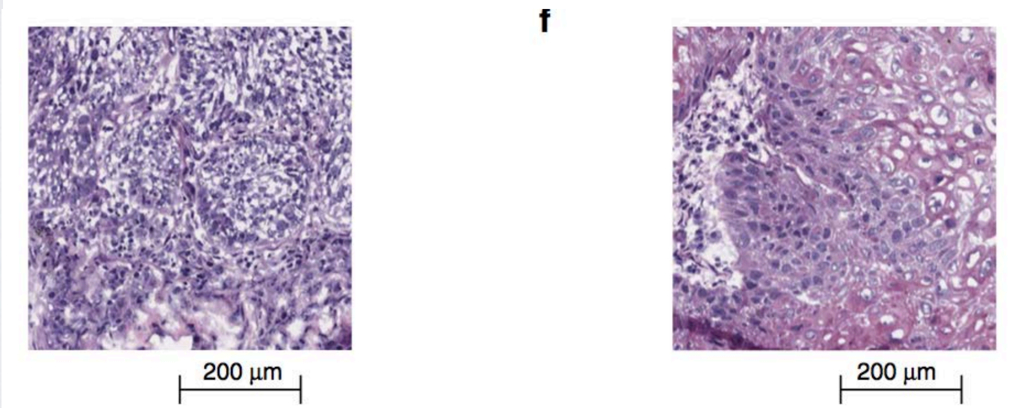
In an edited excerpt from his new book, Too Big to Know, David Weinberger explains how the massive amounts of data necessary to deal with complex phenomena exceed any single brain's ability to grasp, yet networked science rolls on.

PREDICTING LUNG CANCER SURVIVAL

- Which patient would you predict has greater survival rate?



Quantitative image features predicted the survival outcomes of stage I lung adenocarcinoma patients.

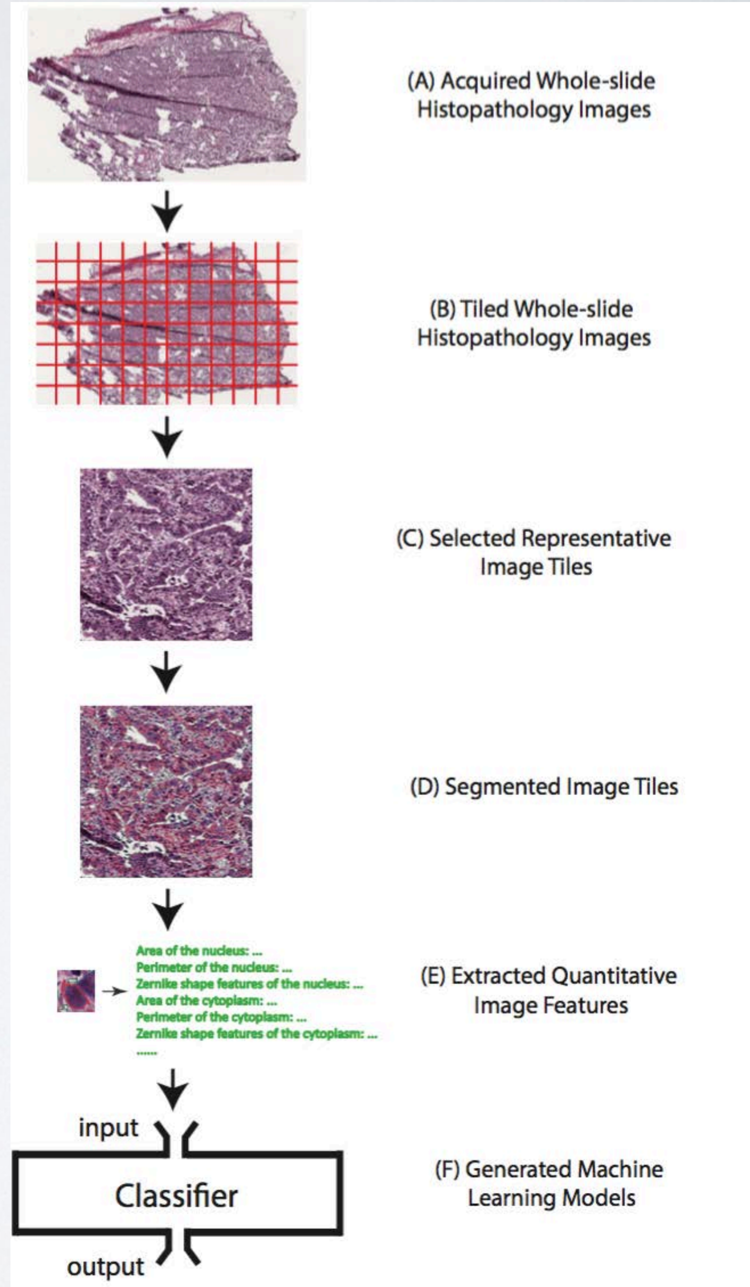


Quantitative image features predicted the survival outcomes of lung squamous cell carcinoma patients.

Predicting non-small cell lung cancer prognosis by fully automated microscopic pathology image features, Nature Comm., 2016, DOI: 10.1038/ncomms12474

MACHINE LEARNING MODELS PREDICT CANCER

- Pathology images acquired
- Place a grid over entire image
- Select a subset of tiles that are "dense"
- Find tumor nuclei and cytoplasm
- Compute quantitative features
- Feed features into a machine learning algorithm (MATH!)



SUMMARY

- Math and computers have opened new opportunities in energy, environment, biology, many more
- Many problems still waiting to be studied
- We need more people with new ideas working on these problems

VISION, COURAGE, …

"All scientific work is incomplete – whether it be observational or experimental. All scientific work is liable to be upset or modified by advancing knowledge. That does not confer upon us a freedom to ignore the knowledge we already have or postpone the action that it appears to demand at a given time"

Bradford Hill, 1965

Living Downstream, pp. 284

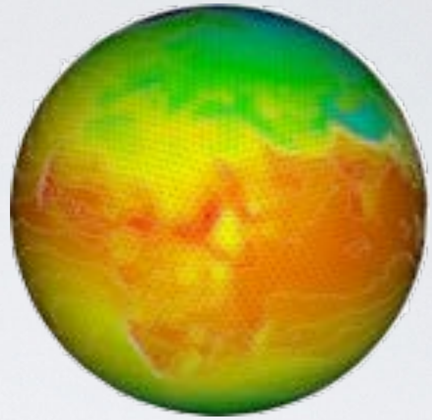
So If Someone Asks You Why You’re Studying Math?

I’m Going To Help Save The World!

SUPPLEMENTAL MATERIALS

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

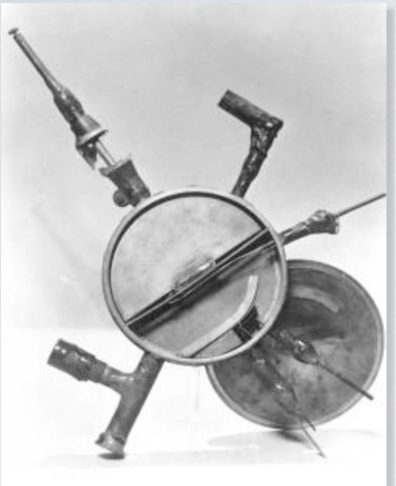
Combustion
Understanding the dispersion of pollutants in the environment.

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

Experiments vs. Computational Science



75,000 increase

4.5 inches diameter

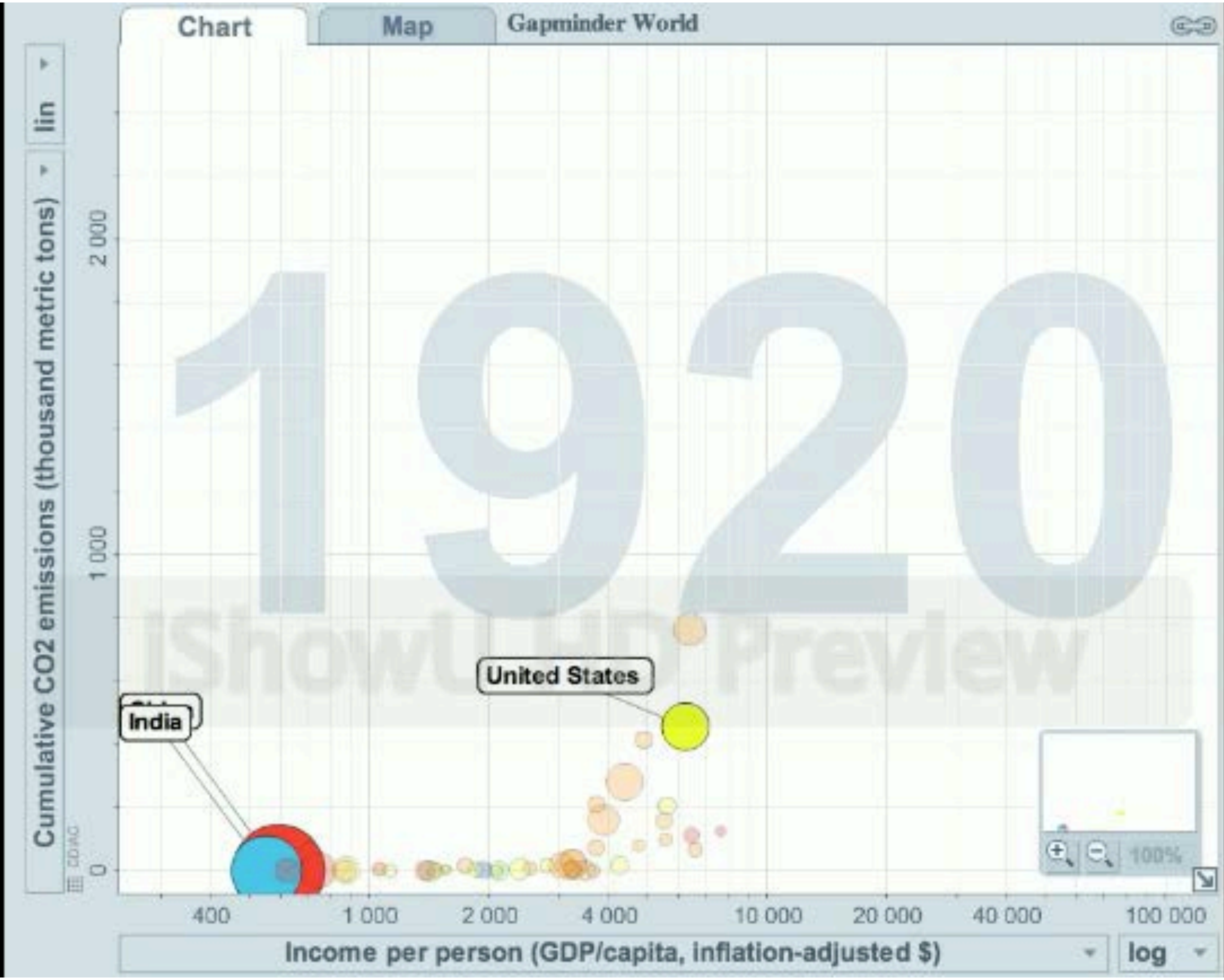
27 km circumference, $4B US

500 Million increase

400 operations/s, $500K

200 Billion operations/s, $400

GAPMINDER
WWW.GAPMINDER.ORG

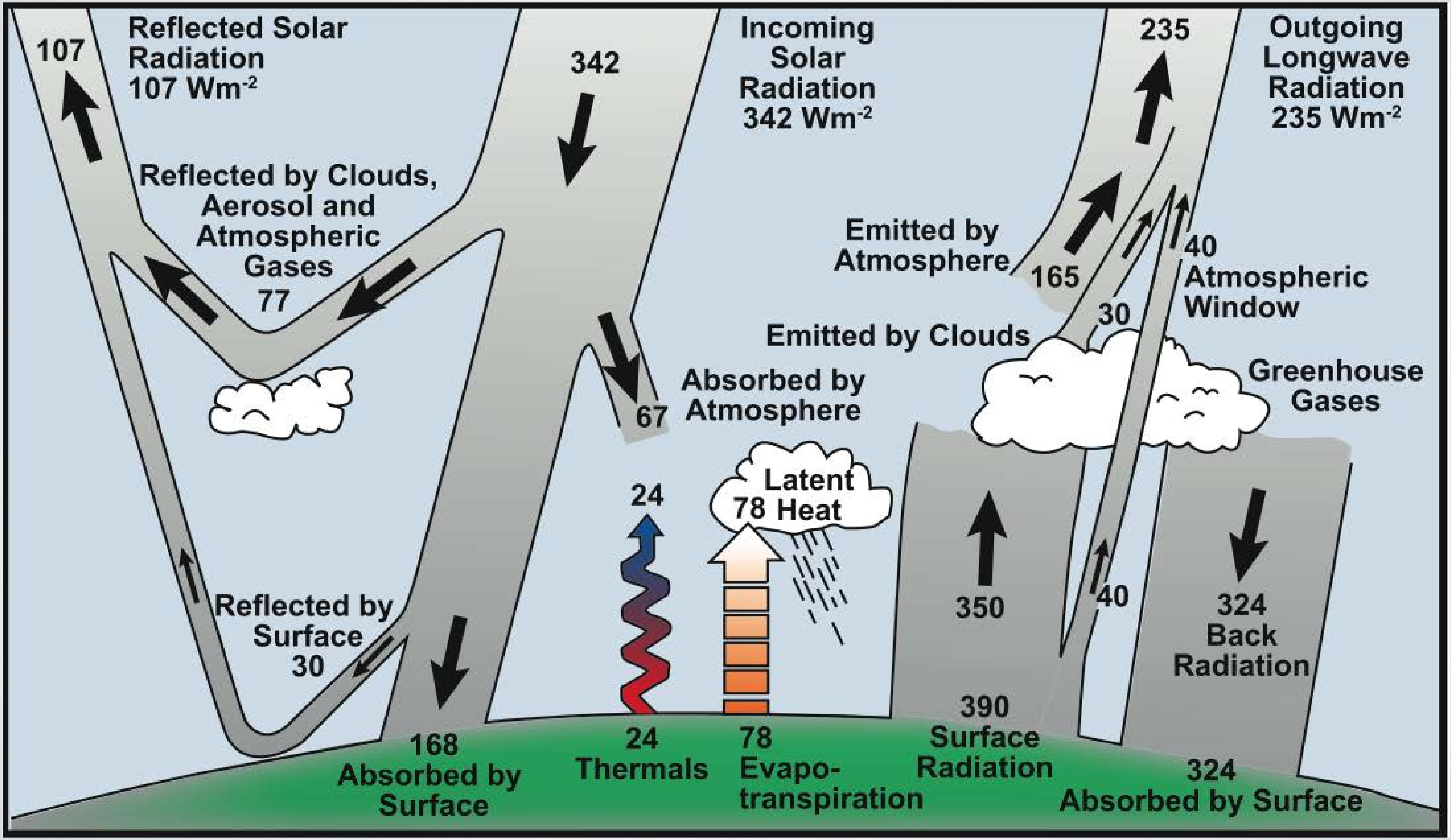


source: gapminder.org

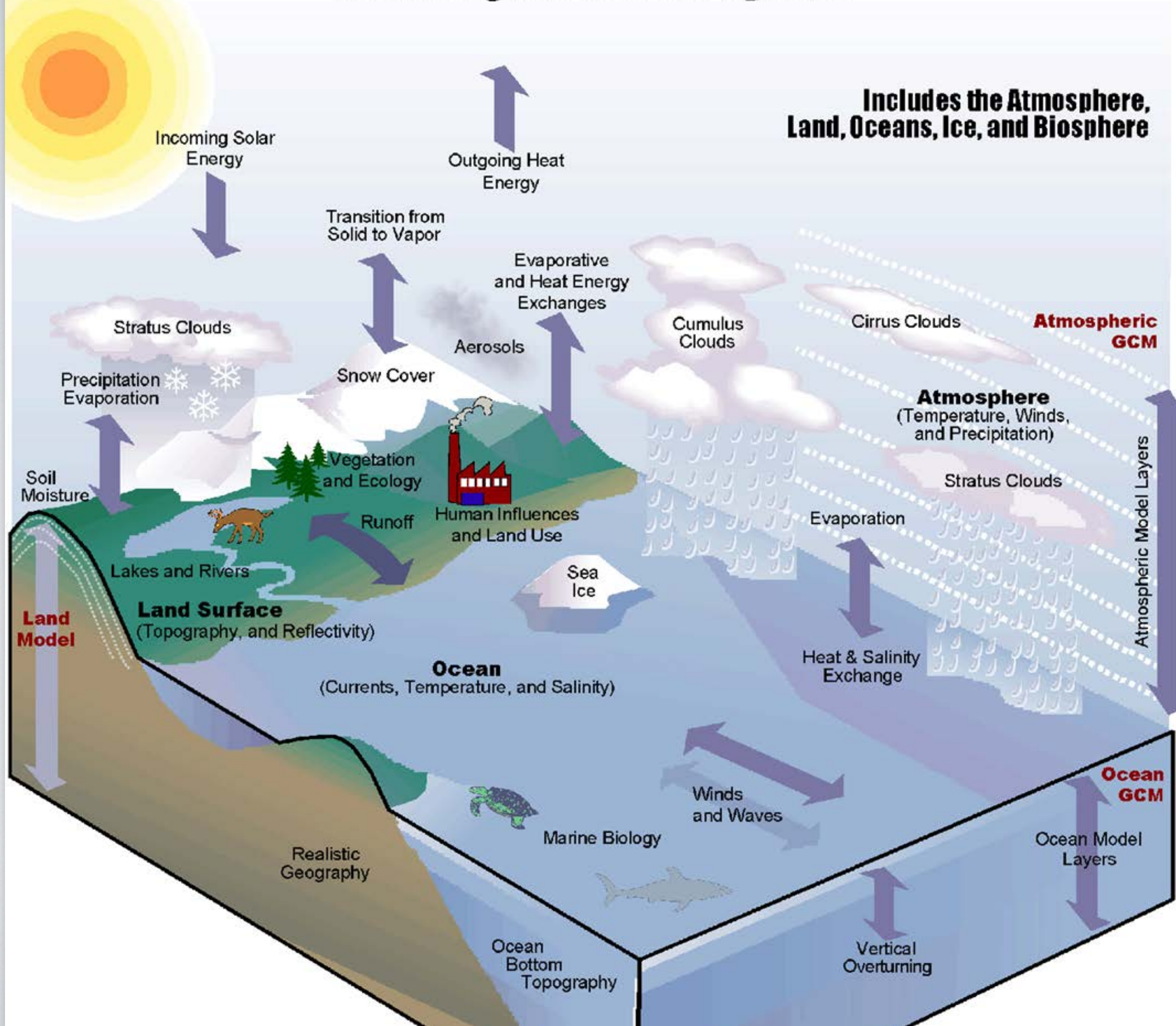
GENERAL CLIMATE

ATMOSPHERE ENERGY BALANCE

$$342 = 107 + 235$$



Modeling the Climate System



Managing the risks: hurricanes in the USA and Caribbean

Risk Factors

- population growth
- increasing property value
- higher storm surge with sea level rise

Risk Management/ Adaptation

- better forecasting
- warning systems
- stricter building codes
- regional risk pooling

Projected globally: *likely* increase in average maximum wind speed and associated heavy rainfall (although not in all regions)

Managing the risks: heat waves in Europe

Risk Factors

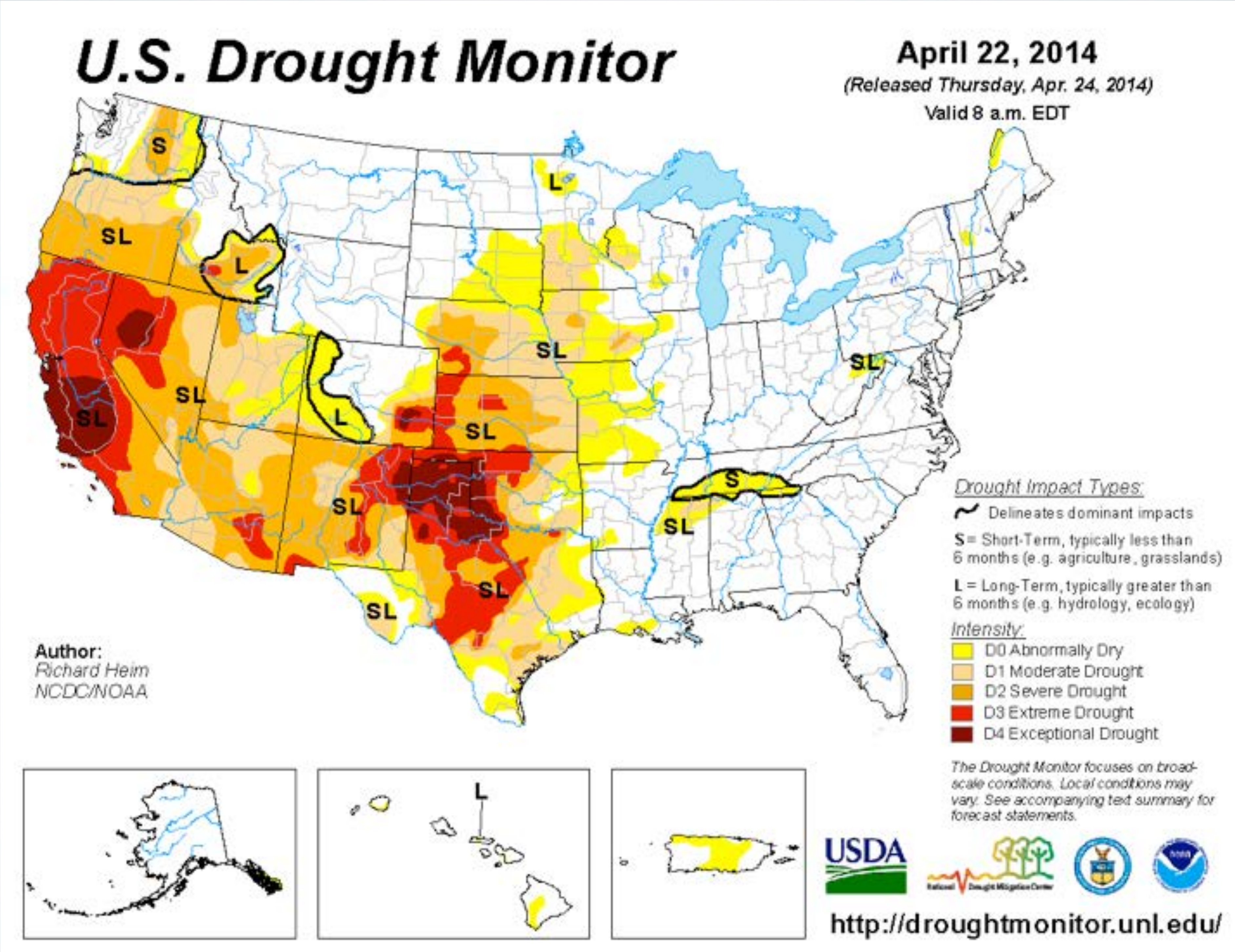
- lack of access to cooling
- age
- pre-existing health problems
- poverty and isolation
- infrastructure

France, August 2003 (over 14,000 dead)

Risk Management/ Adaptation

- cooling in public facilities
- warning systems
- social care networks
- urban green space
- changes in urban infrastructure

Projected: *likely* increase in heat wave frequency and *very likely* increase in warm days and nights across Europe

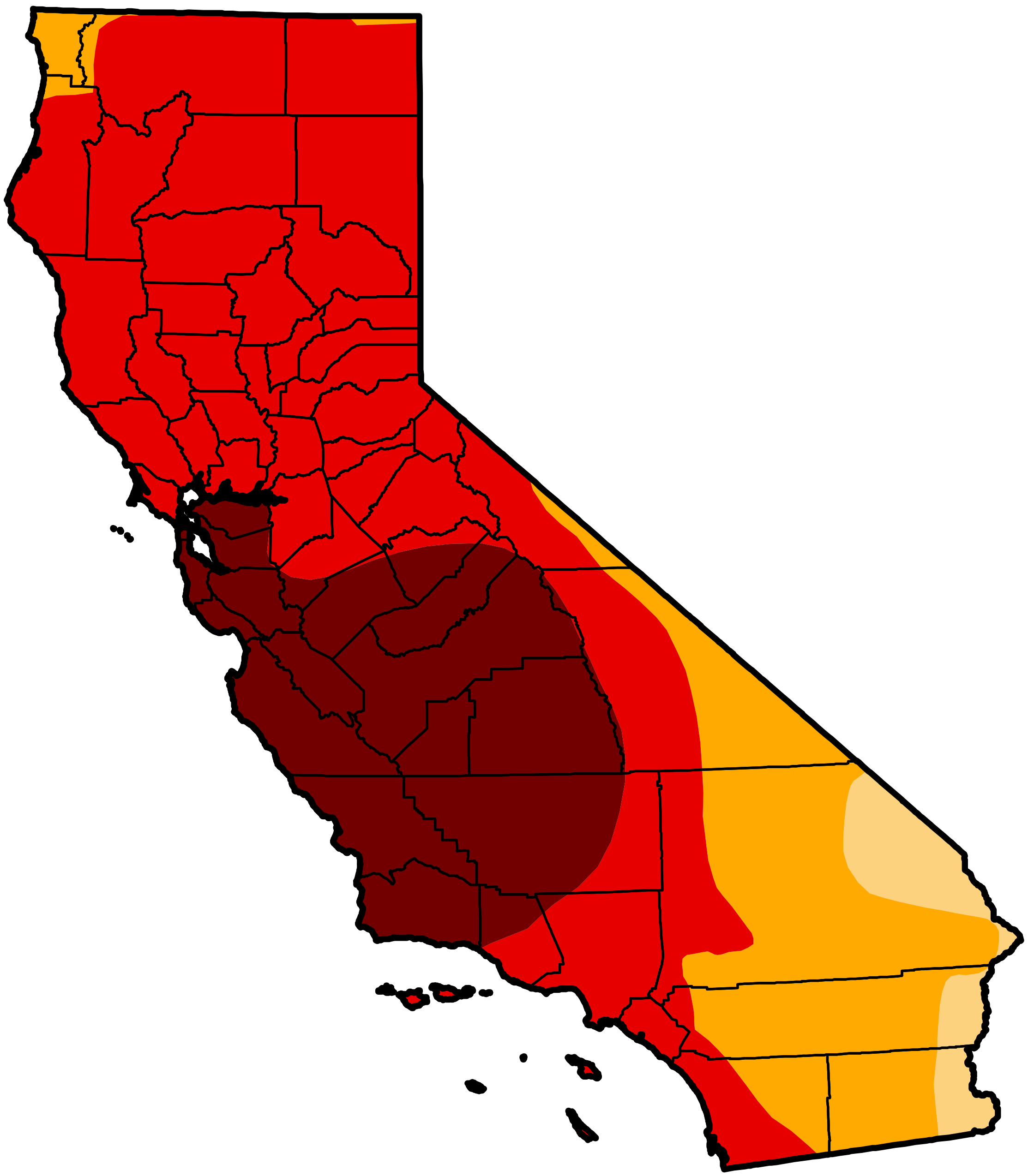

U.S. Drought Monitor
April 22, 2014
(Released Thursday, Apr. 24, 2014)
Valid 8 a.m. EDT
S
L
SL
Drought Impact Types:
Delineates dominant impacts
S = Short-Term, typically less than 6 months (e.g. agriculture, grasslands)
L = Long-Term, typically greater than 6 months (e.g. hydrology, ecology)
Intensity:
D0 Abnormally Dry
D1 Moderate Drought
D2 Severe Drought
D3 Extreme Drought
D4 Exceptional Drought
Author:
Richard Heim
NCDC/NOAA
The Drought Monitor focuses on broad-scale conditions. Local conditions may vary. See accompanying text summary for forecast statements.
USDA
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
- 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 — National Drought Mitigation Center

http://droughtmonitor.unl.edu/

U.S. Drought Monitor

California

April 21, 2015

(Released Thursday, Apr. 23, 2015)

Valid 7 a.m. EST

Drought Conditions (Percent Area)

	None	D0-D4	D1-D4	D2-D4	D3-D4	D4
Current	0.14	99.86	98.11	93.44	66.60	46.77
Last Week *4/14/2015*	0.14	99.86	98.11	93.44	66.60	44.32
3 Months Ago *1/20/2015*	0.00	100.00	98.13	94.34	77.52	39.15
Start of Calendar Year *12/30/2014*	0.00	100.00	98.12	94.34	77.94	32.21
Start of Water Year *9/30/2014*	0.00	100.00	100.00	95.04	81.92	58.41
One Year Ago *4/22/2014*	0.00	100.00	100.00	96.01	76.68	24.77

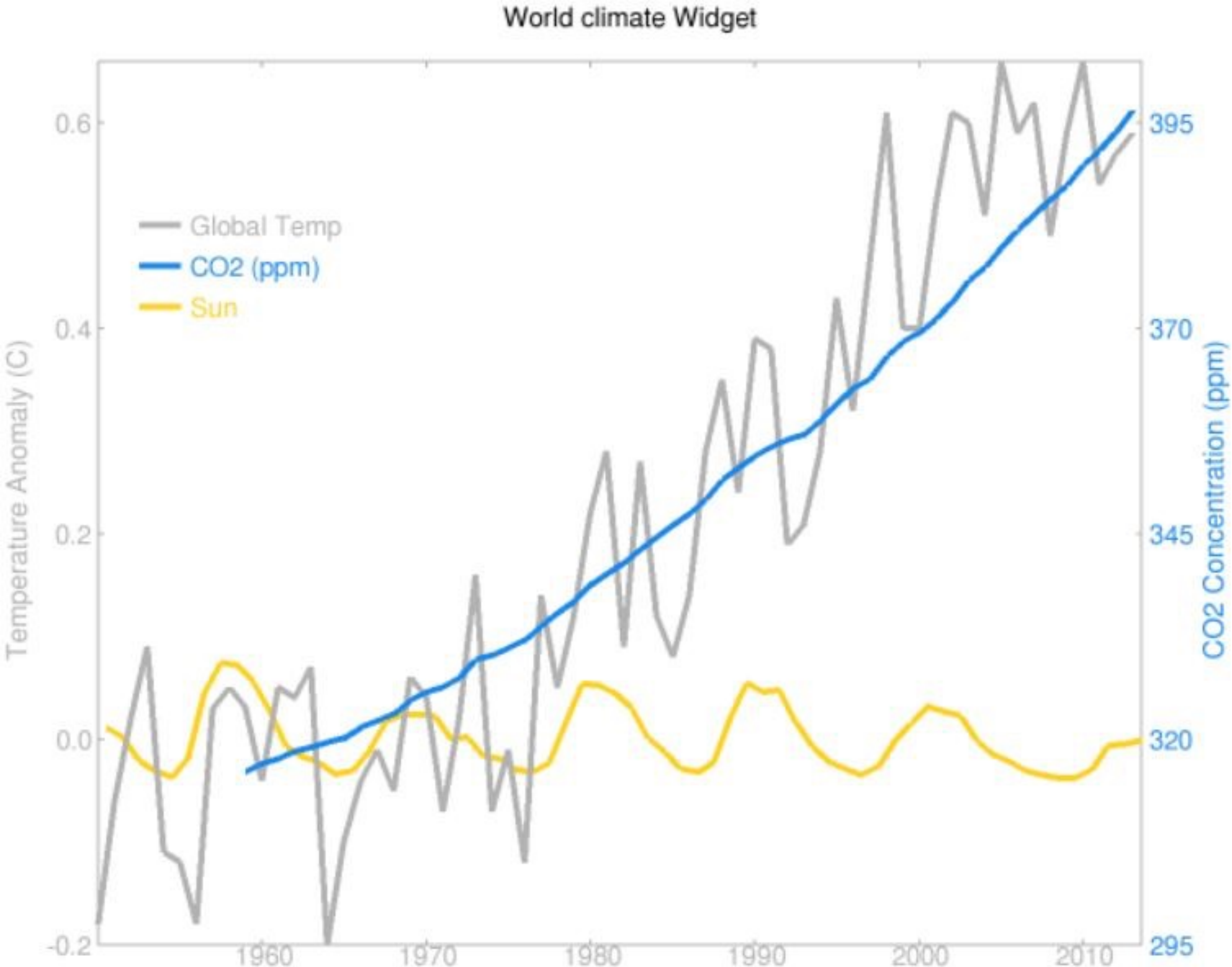
Intensity:

- 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:
Anthony Artusa
NOAA/NWS/NCEP/CPC

http://droughtmonitor.unl.edu/



http://herdsoft.com/climate/widget/

BIOFUELS

IF BURNING FOSSIL FUELS IS BAD WHAT ARE THE ALTERNATIVES?

Biofuels

Solar Energy

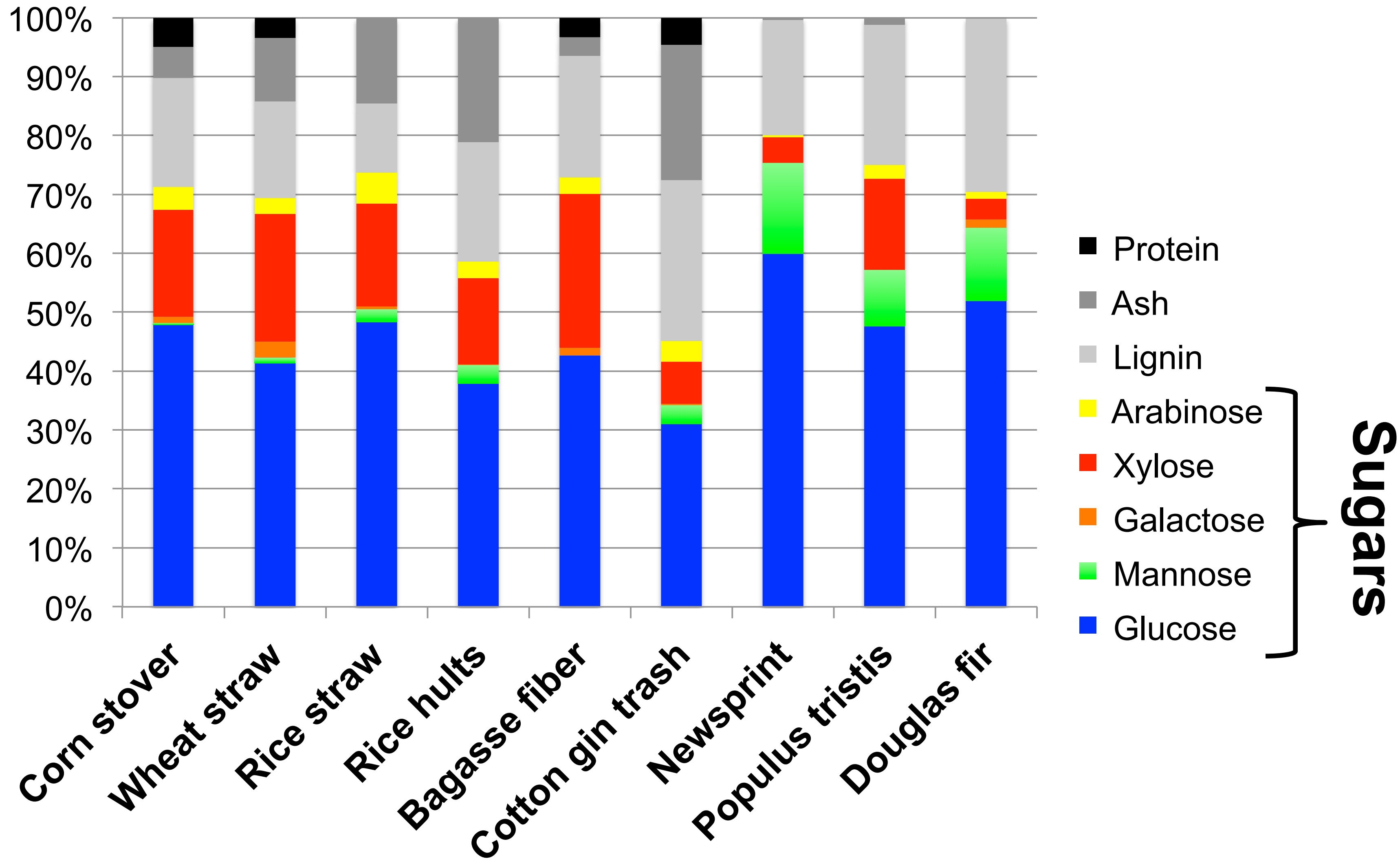
Wind

BIOFUELS

PHOTOGRAPH COURTESY USDA-ARS VIA PNAS

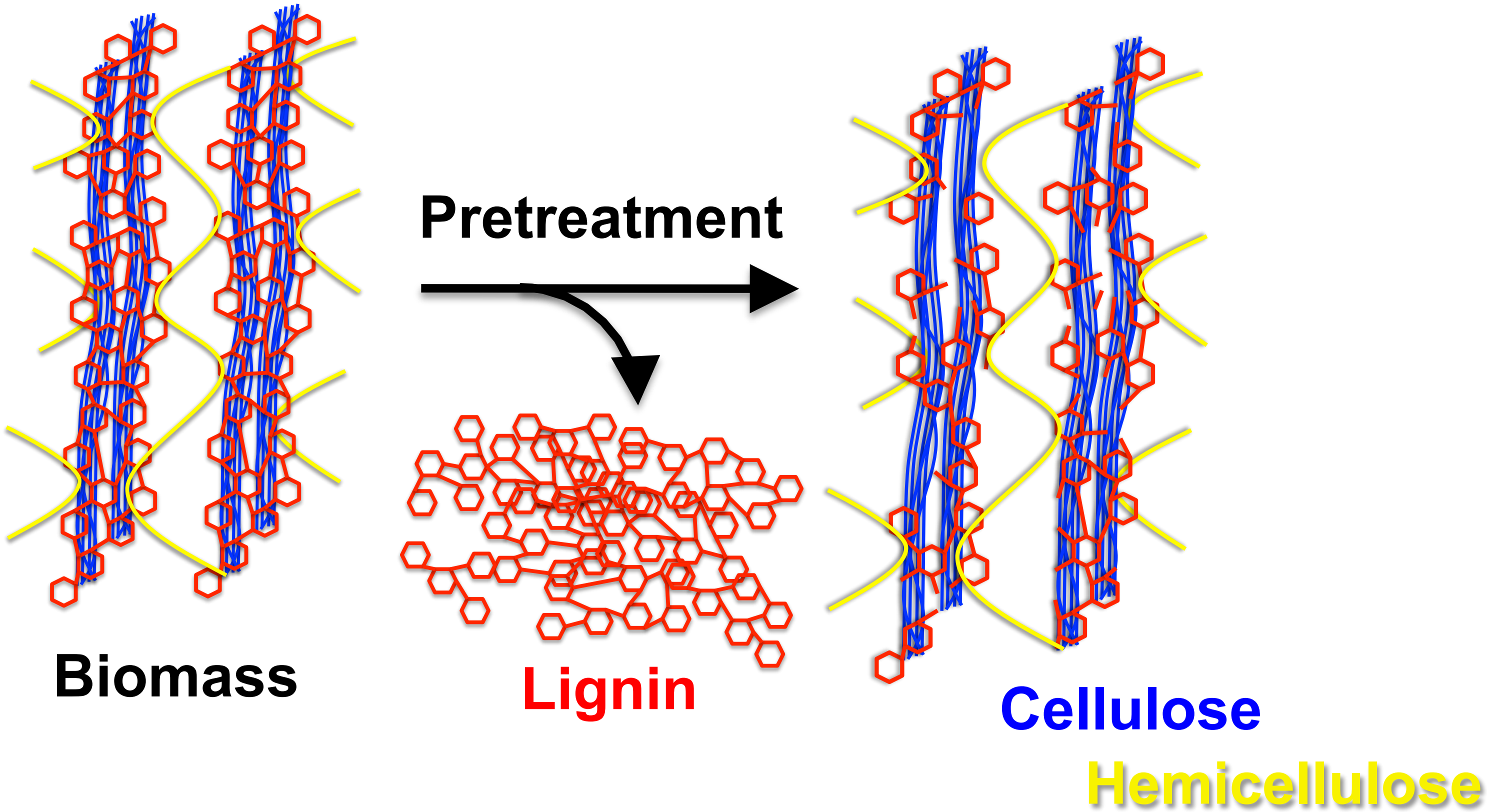
- Idea – Convert sugars in plants into a fuel
- Plants have evolved to be resistant to physical and chemical attack
- If we can understand plant genomics better could we develop better biofuels?

Biomass is predominantly sugar!



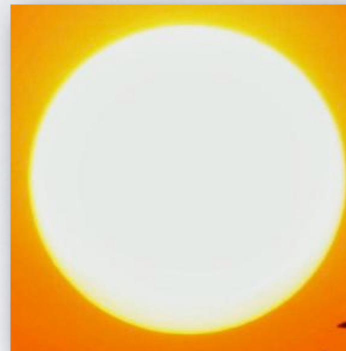
Courtesy of Dr. Jay Keasling, LBNL/UCB

BIOFUELS ARE DERIVED FROM THE SUGARS



Courtesy of Dr. Jay Keasling, LBNL/UCB

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

Math Can Also be Used to Find Drought Resistant Plants

The loss of harvests in the world's dry areas could have a significant impact on global food security

Researchers are developing mathematical models to identify genetic material that could help improve food crops' resilience to climate change.

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].

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

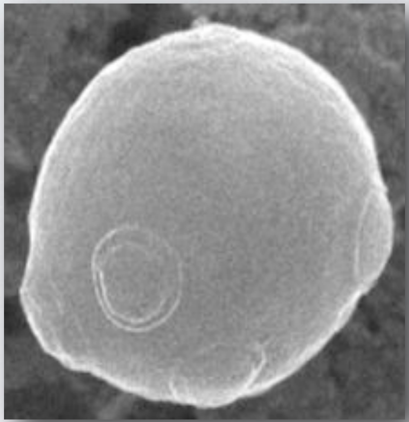
Start-Up Uses Plant Seeds for a Biofuel, By TODD WOODY, New York Times, December 24,

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

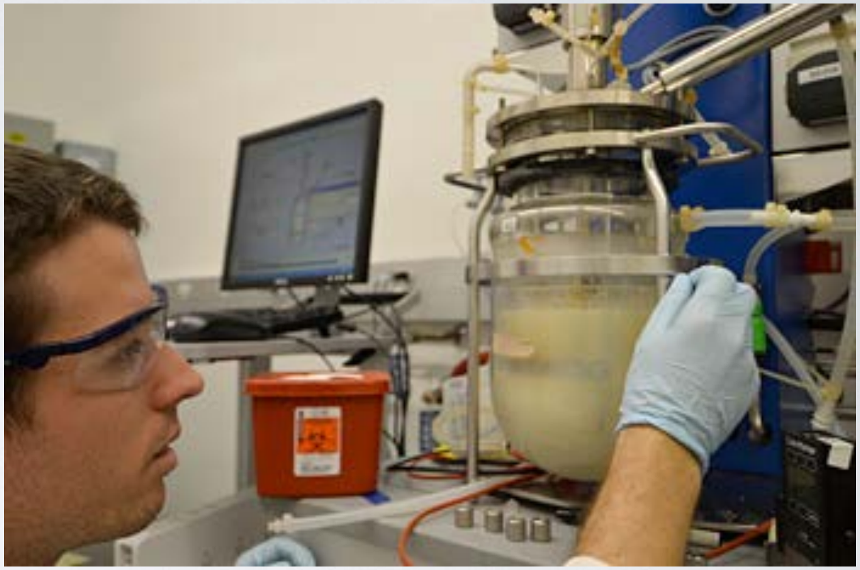
CHALLENGES STILL EXIST FOR BIOFUELS



- Design of plants that have more sugars with less lignin
- Need better processes for producing the sugars
- Many different types of fuels

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



***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