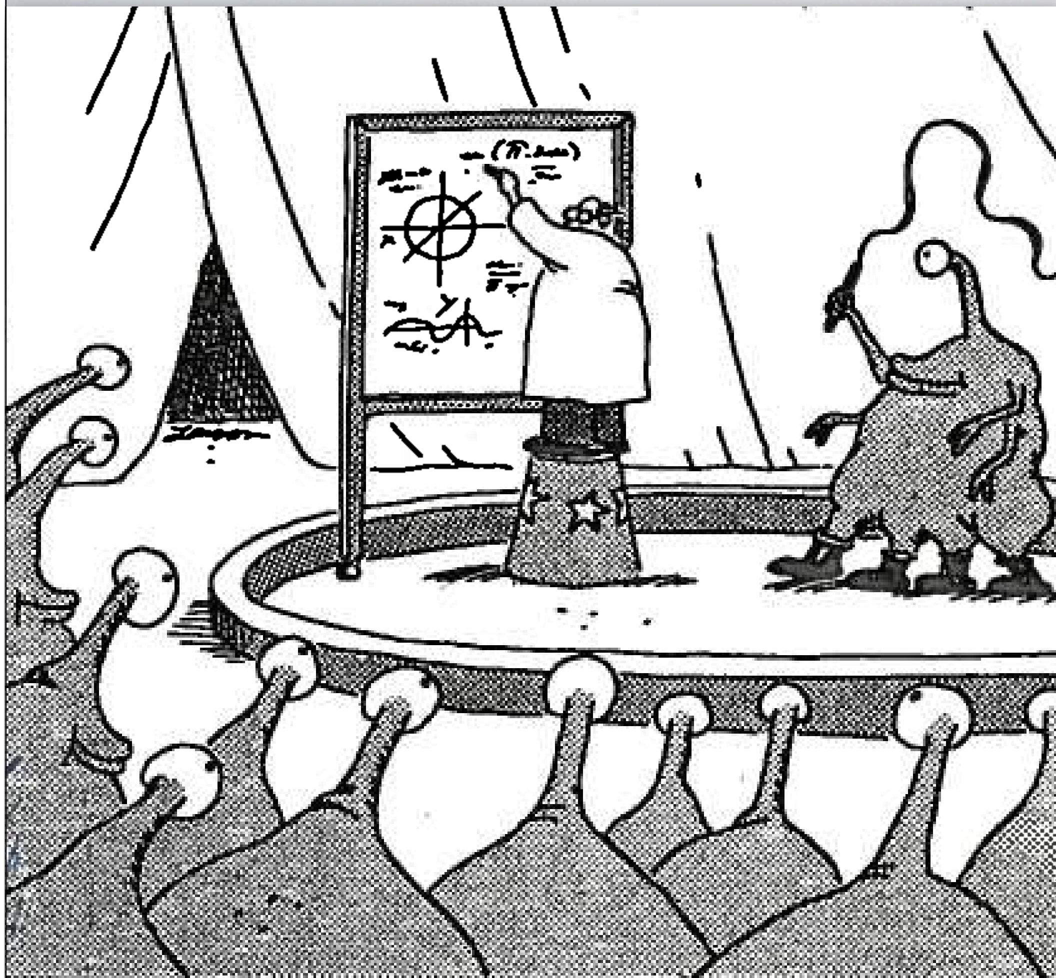
Computational Math and Science

How Mathematics Will Help Save The World

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

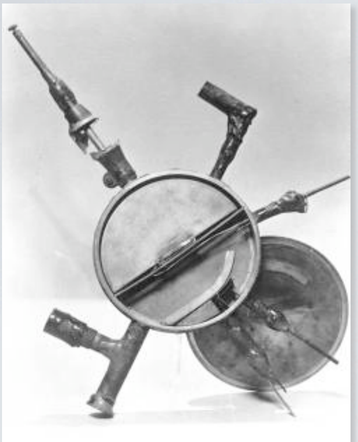
Questions that I am often asked



Abducted by an alien circus company, Professor Doyle is forced to write calculus equations in center ring.

- What is computational science?
- How can science and math help us solve energy problems?
- Can I really make a living as a mathematician?

Experiments vs. Computational Science

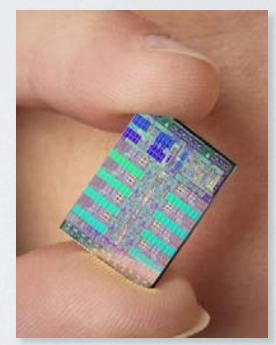


75,000 increase

4.5 inches diameter

27 km circumference, $4B US

500 Million increase

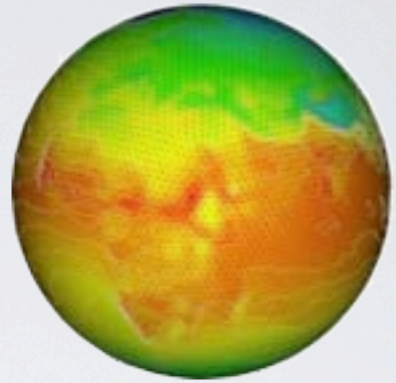


400 operations/s, $500K

200 Billion operations/s, $400

Unprecedented Progress

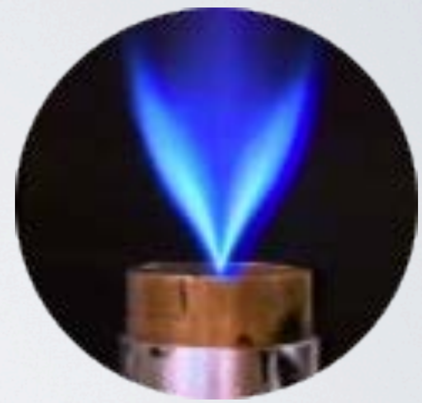
Energy Efficiency
Tools for predicting building energy use



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.

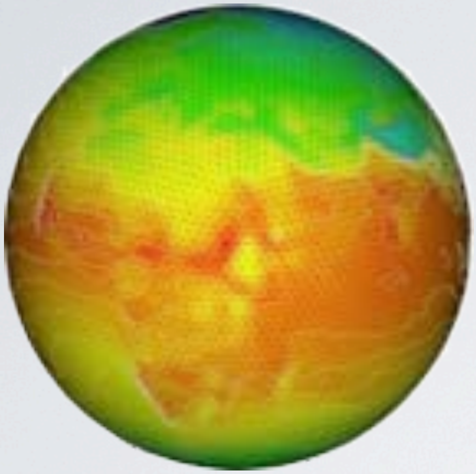


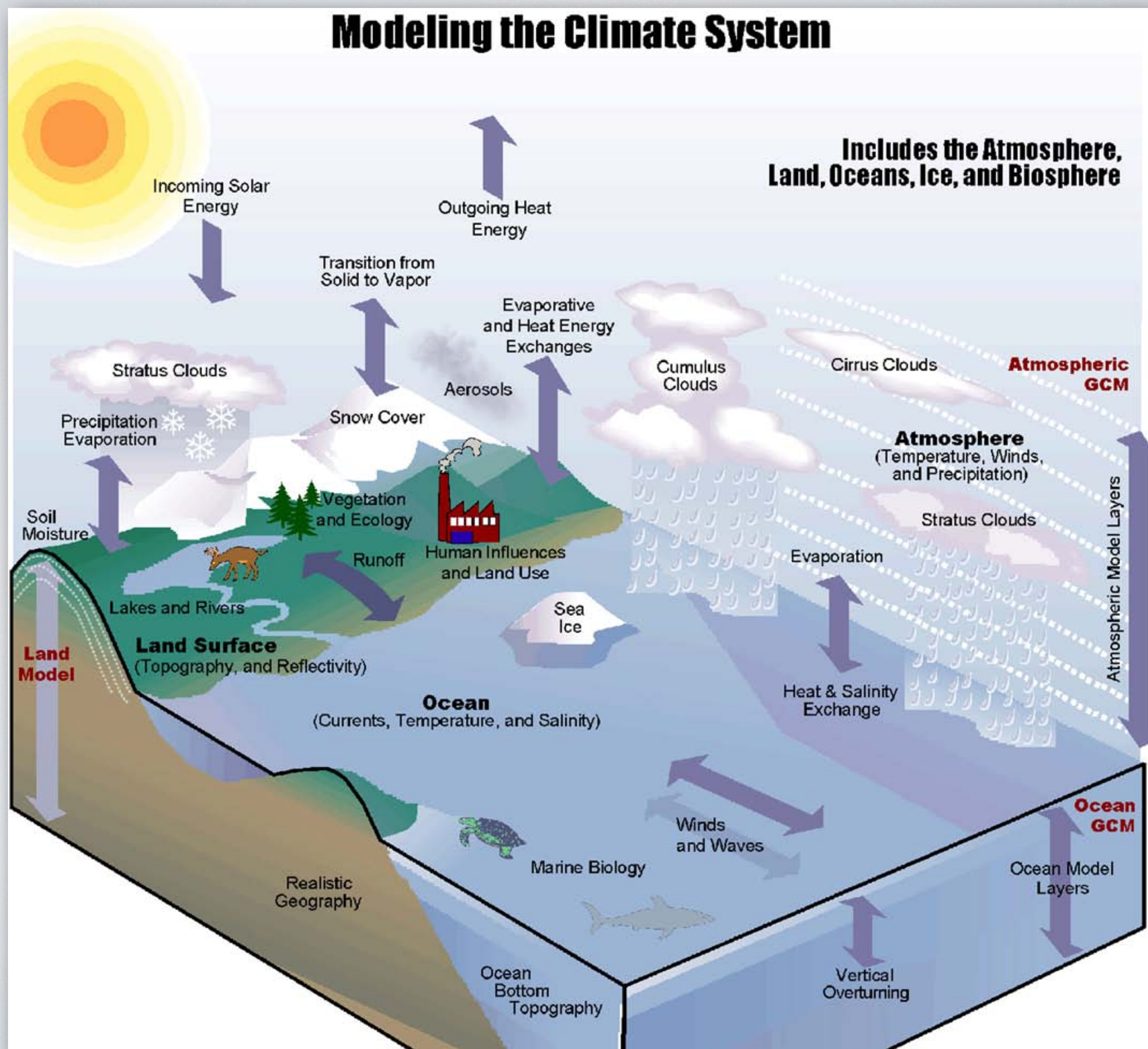
Biofuels
Simulation models for understanding bottlenecks to economical biofuels

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

Images courtesy of Lawrence Berkeley National Laboratory

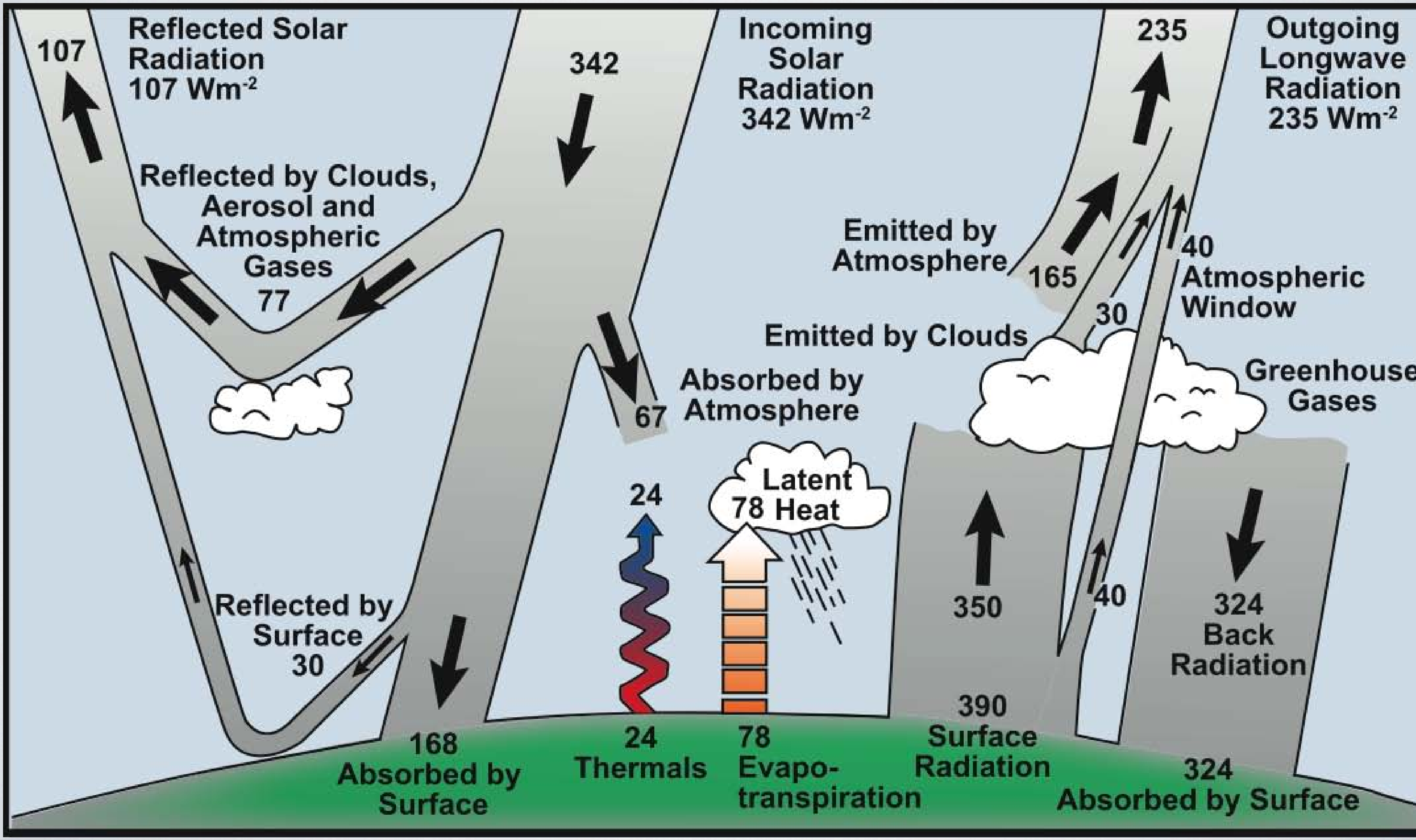
What is a Climate Model?




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
Aerosols
Cumulus Clouds
Cirrus Clouds
Atmospheric GCM
Precipitation Evaporation
Snow Cover
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

ATMOSPHERE ENERGY BALANCE

$342 = 107 + 235$



FIRST MENTION OF GREENHOUSE EFFECT

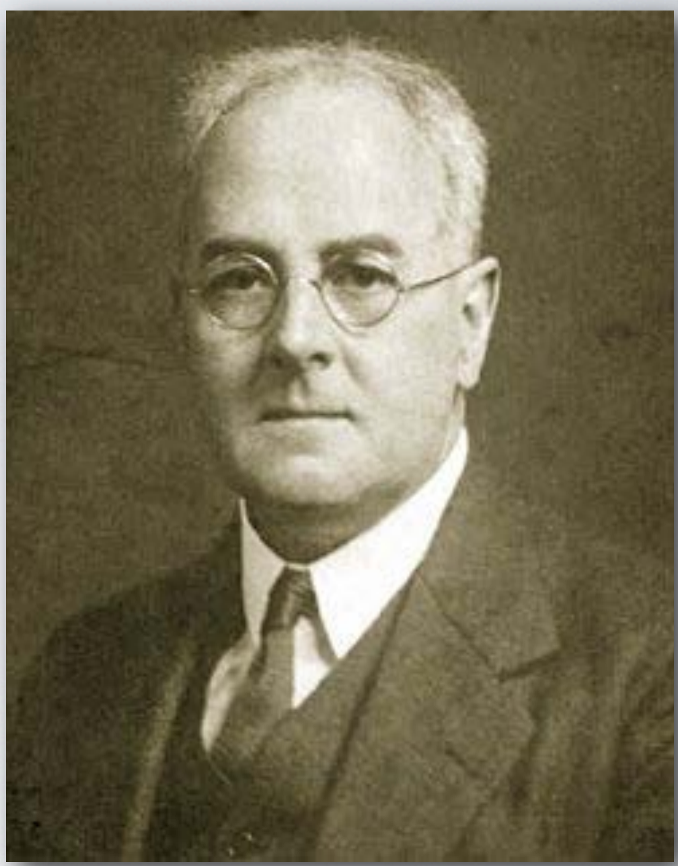
- Developed mathematical theory for the temperature of the terrestrial globe

- “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

PRIMITIVE EQUATIONS FOR ATMOSPHERE

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

Conservation of momentum

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

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

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

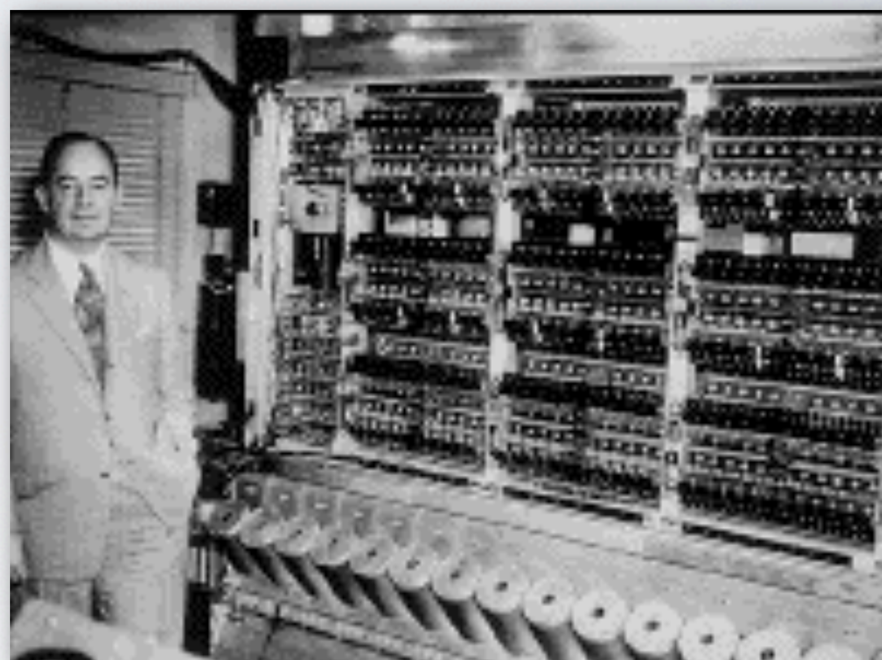
$$C_p\frac{dT}{dt} - \frac{1}{\rho}\frac{dp}{dt} = Q$$

Equation of state

$$p = \rho RT$$

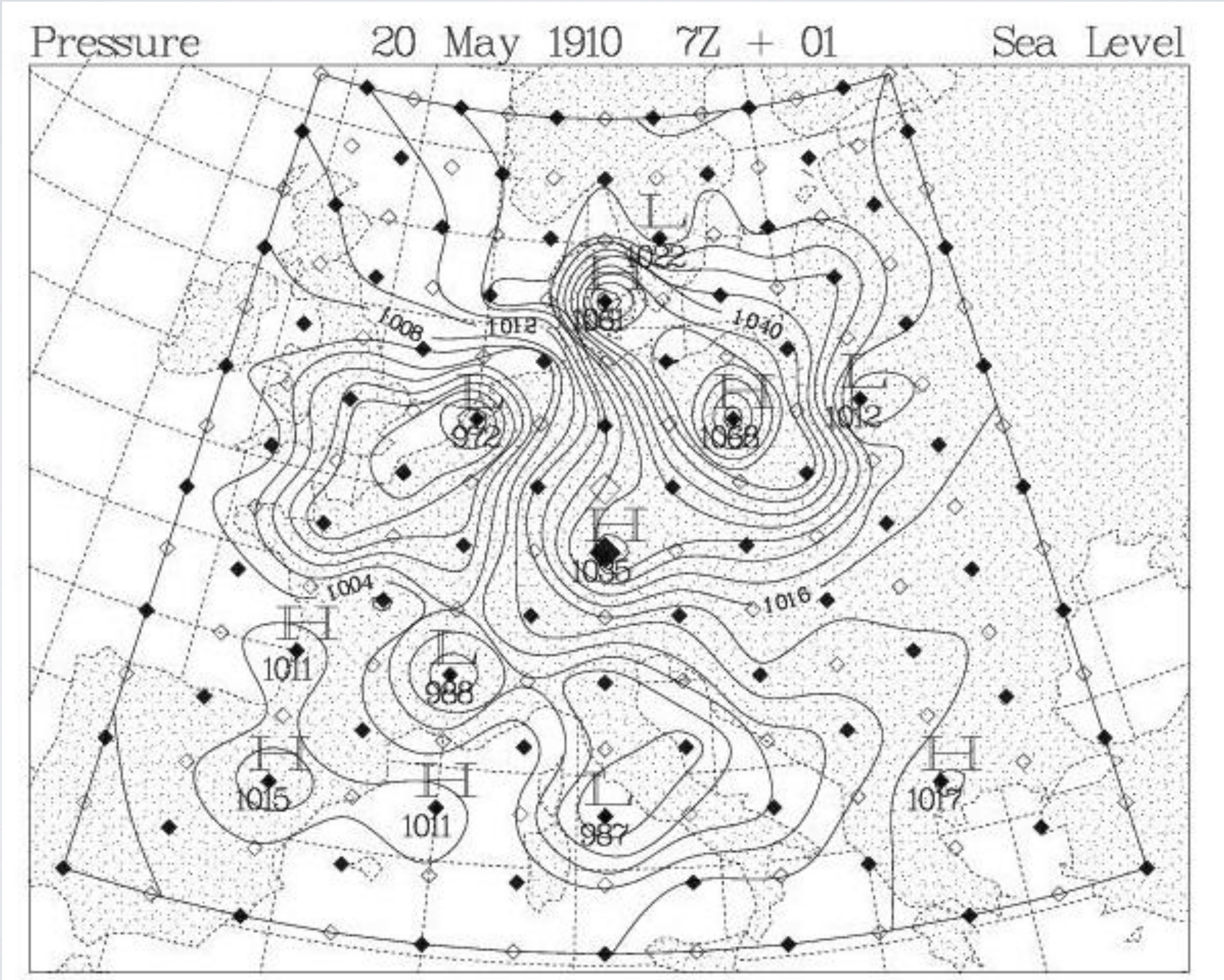
JOHN VON NEUMANN'S METEOROLOGY PROJECT

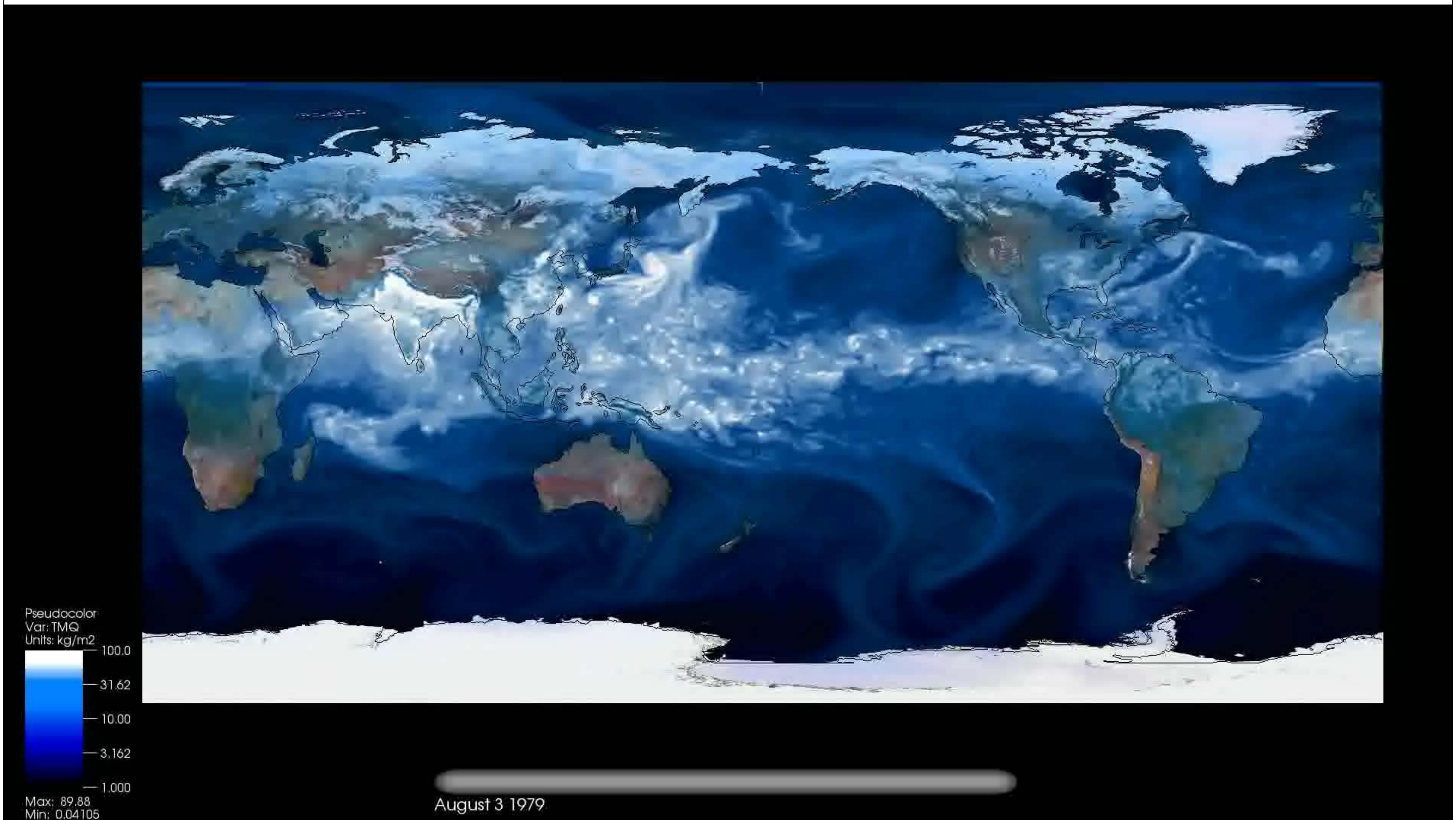
- Recognized numerical weather forecasting as a problem of great importance
- In collaboration with Charney and Fjortoft, they completed the first numerical computer forecast in 1950
- Used ENIAC, first multipurpose electronic digital computer
- Each 24 hour forecast took 24 hours to compute



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

RICHARDSON'S COMPUTATION



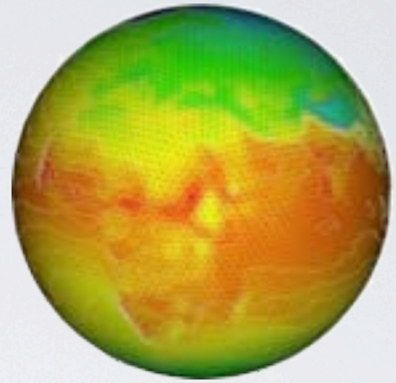


Movie courtesy of W. Washington, NCAR

Unprecedented Progress

Energy Efficiency

Tools for predicting building energy use



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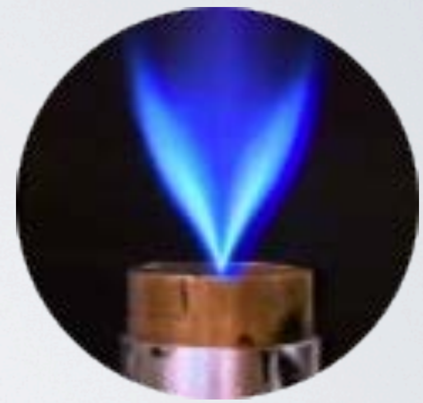


Biofuels

Simulation models for understanding bottlenecks to economical biofuels

Nano Science

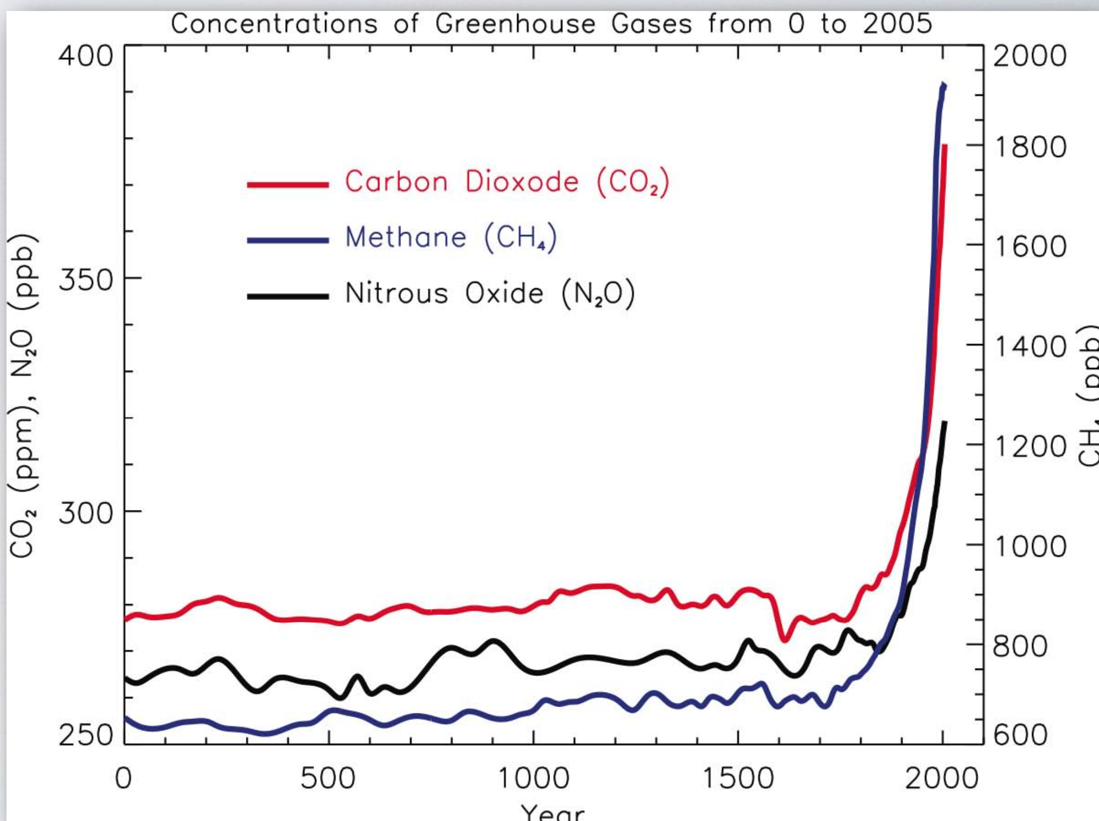
Predicting properties of next-generation photovoltaic solar cell materials.

Combustion

85% of our energy comes from the burning of fossil fuels

ANNUAL GLOBAL RELEASE OF CARBON IS 9 BILLION TONS

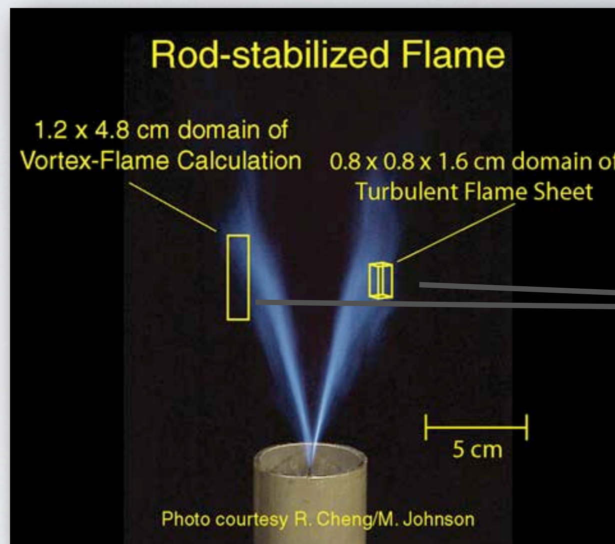
- In US, combustion
  - Transportation
  - Power generation
- 40% coal, 40% oil, 20% natural gas
- US consumes (per day):
  - 20 million barrels of oil
  - 60 billion cubic feet natural gas
  - 3 million tons of coal



Climate Change 2007, The Physical Science Basis, Working Group 1, Solomoon, Qin, Manning ed.

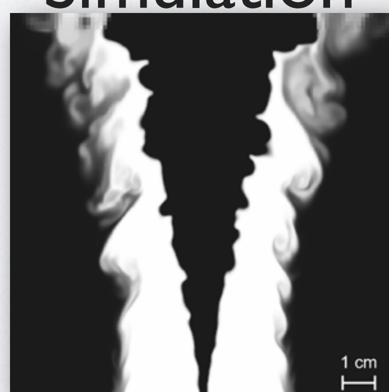
INCREASING COMBUSTION EFFICIENCY CAN REDUCE GREENHOUSE GASES

- New systems are based on *lean premixed turbulent combustion* because they are more efficient and have low emissions
- Challenges
  - Natural flame instabilities
  - Sensitivity to fuel
- Advances in applied math have increased our ability to simulate real systems

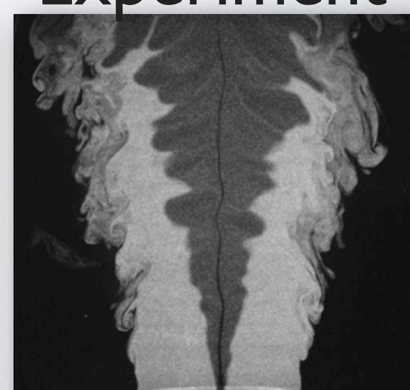


Before

Simulation



Experiment



LOW MACH NUMBER EQUATIONS

$$\rho \frac{DU}{Dt} = -\nabla \pi + \nabla \cdot \tau$$ *momentum*

$$\frac{\partial \rho Y_m}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$ *species*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$ *mass*

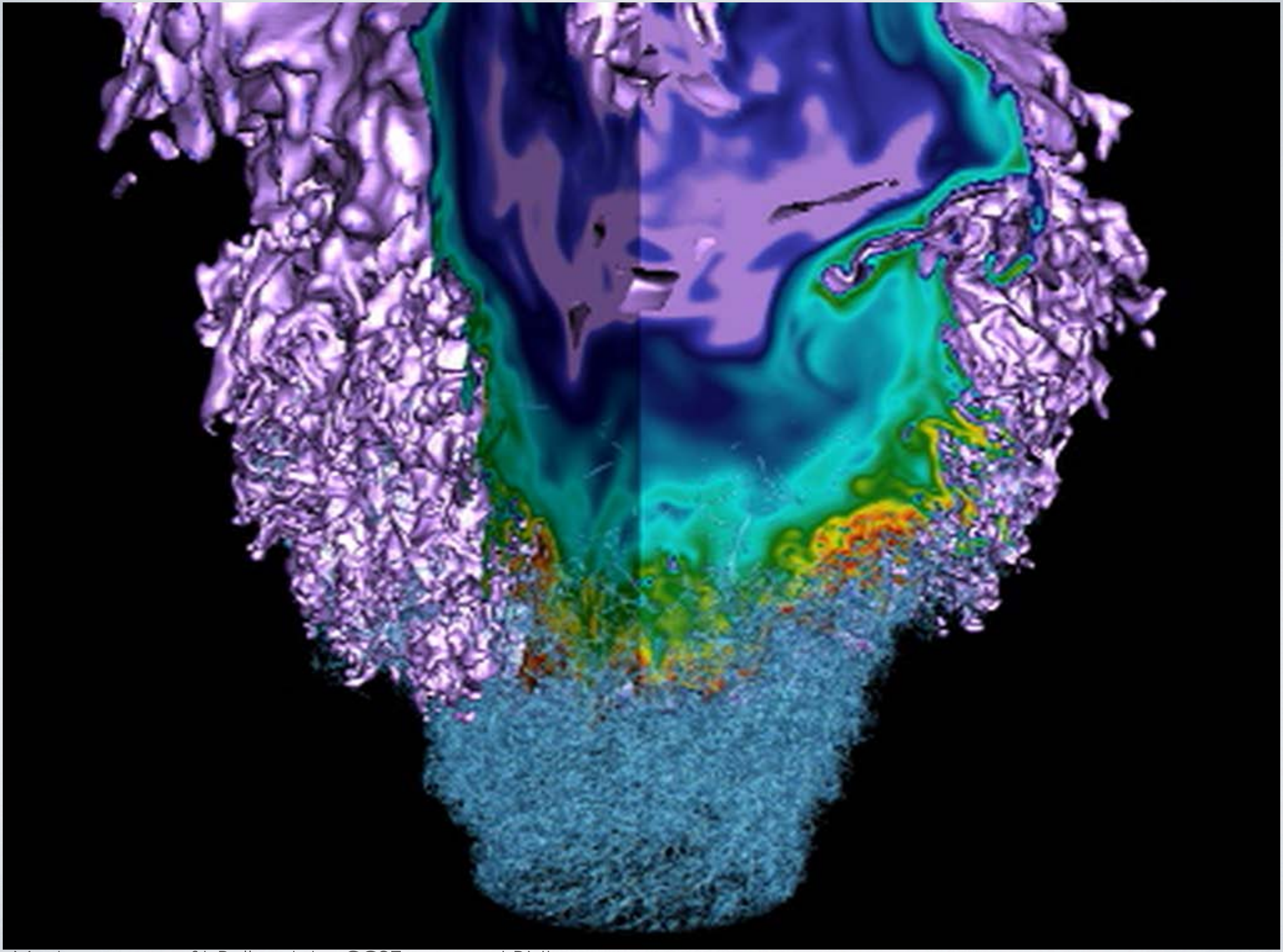
$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h U) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$ *energy*

Y_m mass fraction

$\dot{\omega}_m$ species production, $\sum \dot{\omega}_m = 0$

h enthalpy, $h = \sum Y_m h_m(T)$

Equation of State $p_0 = \rho R T \sum Y_m / W_m$ *equation of state*



Movie courtesy of J. Bell and the CCSE group at LBNL

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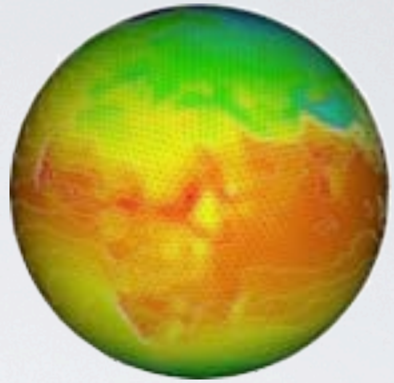

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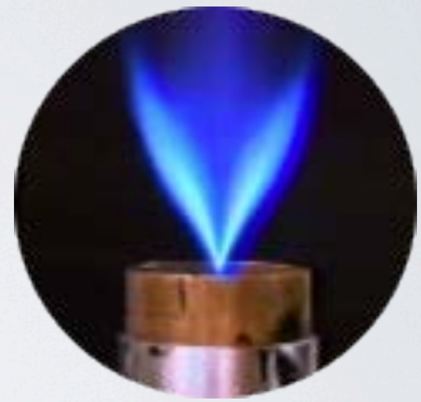

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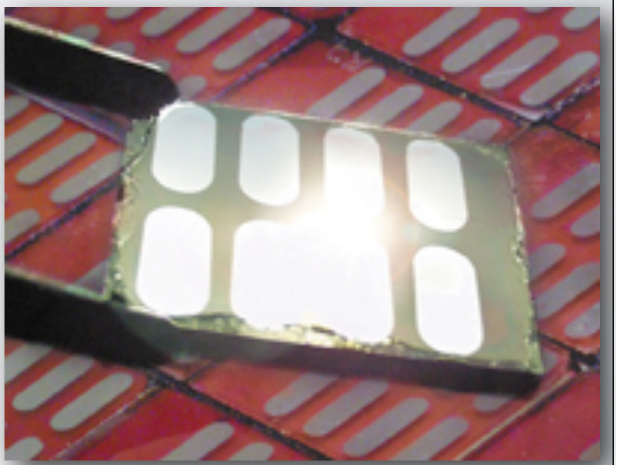
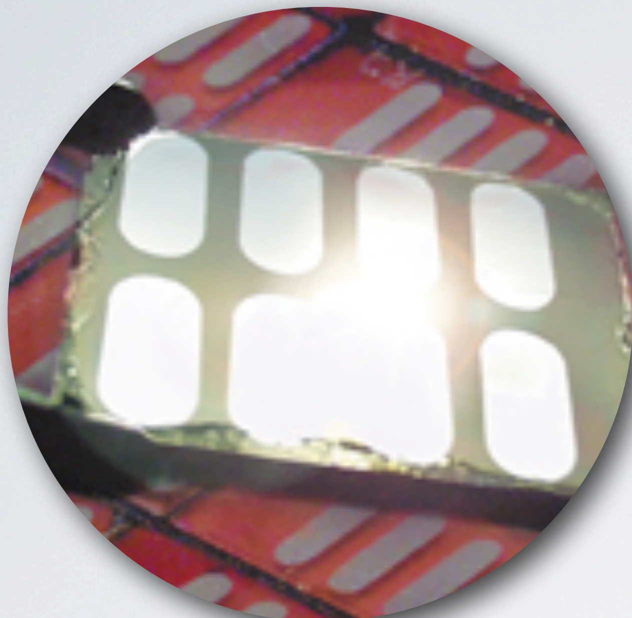
Solar Photo Voltaics

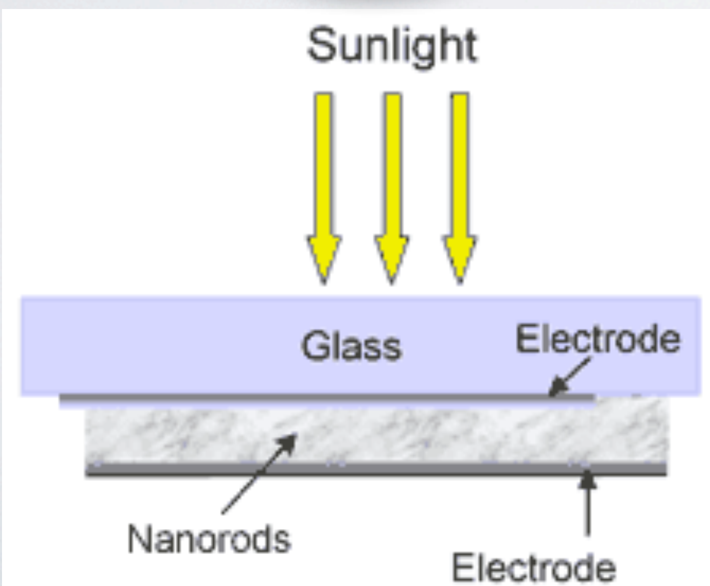
Global Annual Solar Resource: 8.9×10^{8} TWh

Global Annual Electricity Usage: 1.7×10^{4} TWh



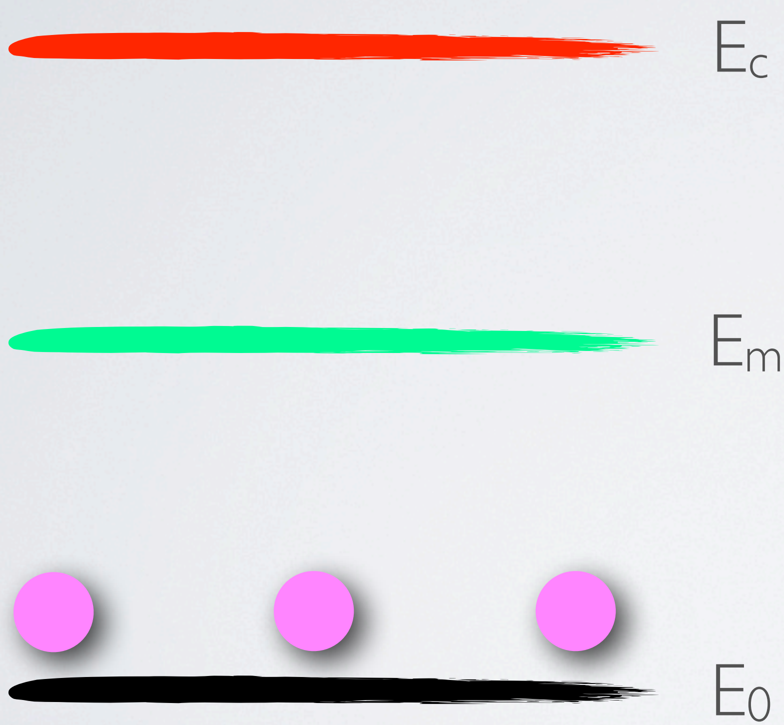
PHOTOVOLTAIC SOLAR CELLS





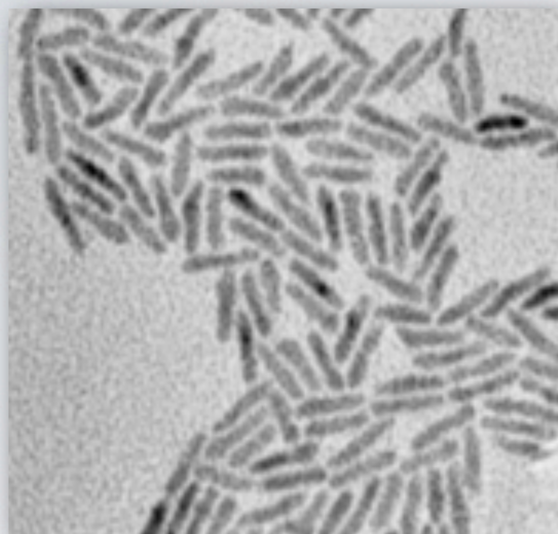
- Solar cells based on nanorods
- Nanorods can be made of CdSe, a semiconducting material
- Nanorods act like wires, absorbing light and generating electricity
- Biggest challenge is cost, ~30 cents/kWh

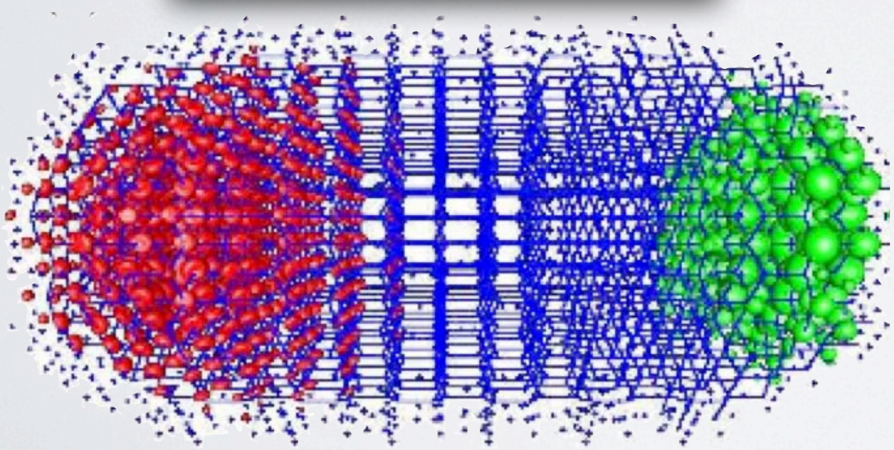
CAN WE DESIGN MATERIALS WITH IMPROVED SOLAR CELL EFFICIENCY?



- Best predicted efficiency is 30% if one material is used
- Can we do better using two or more materials
- What's the right mix of materials?

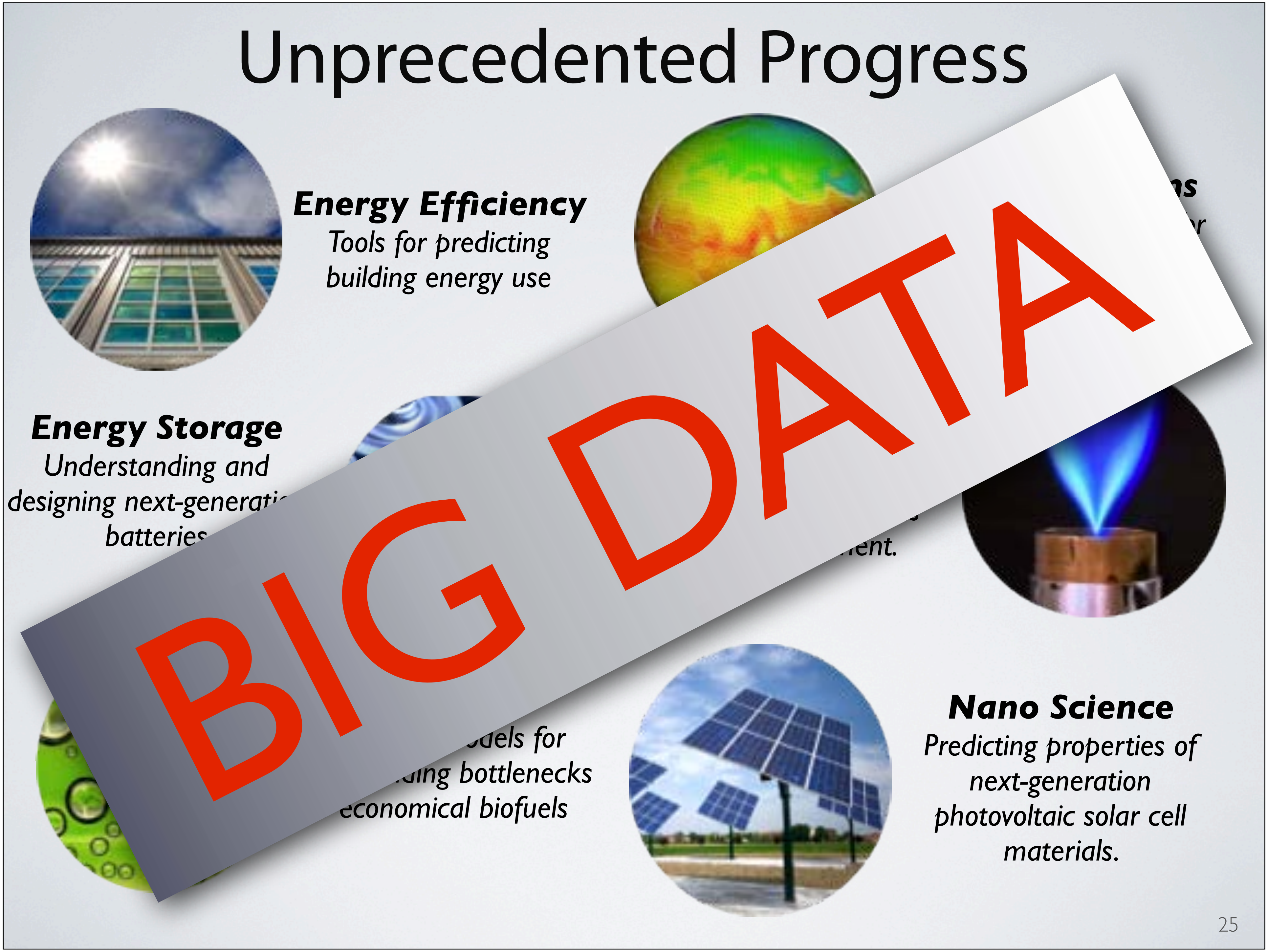
CALCULATIONS HELP TO EXPLAIN EXPERIMENTS





Linear-scaling three-dimensional fragment method for large-scale electronic structure calculations, Wang, Zhao, Meza, doi: 10.1103/PhysRevB.77.165113, April 2008.

- Experiments show that these structures have good properties
- Need to compute the structure for 2633 atom molecule
- Using 2560 processors at NERSC, the calculation took about 30 hours.



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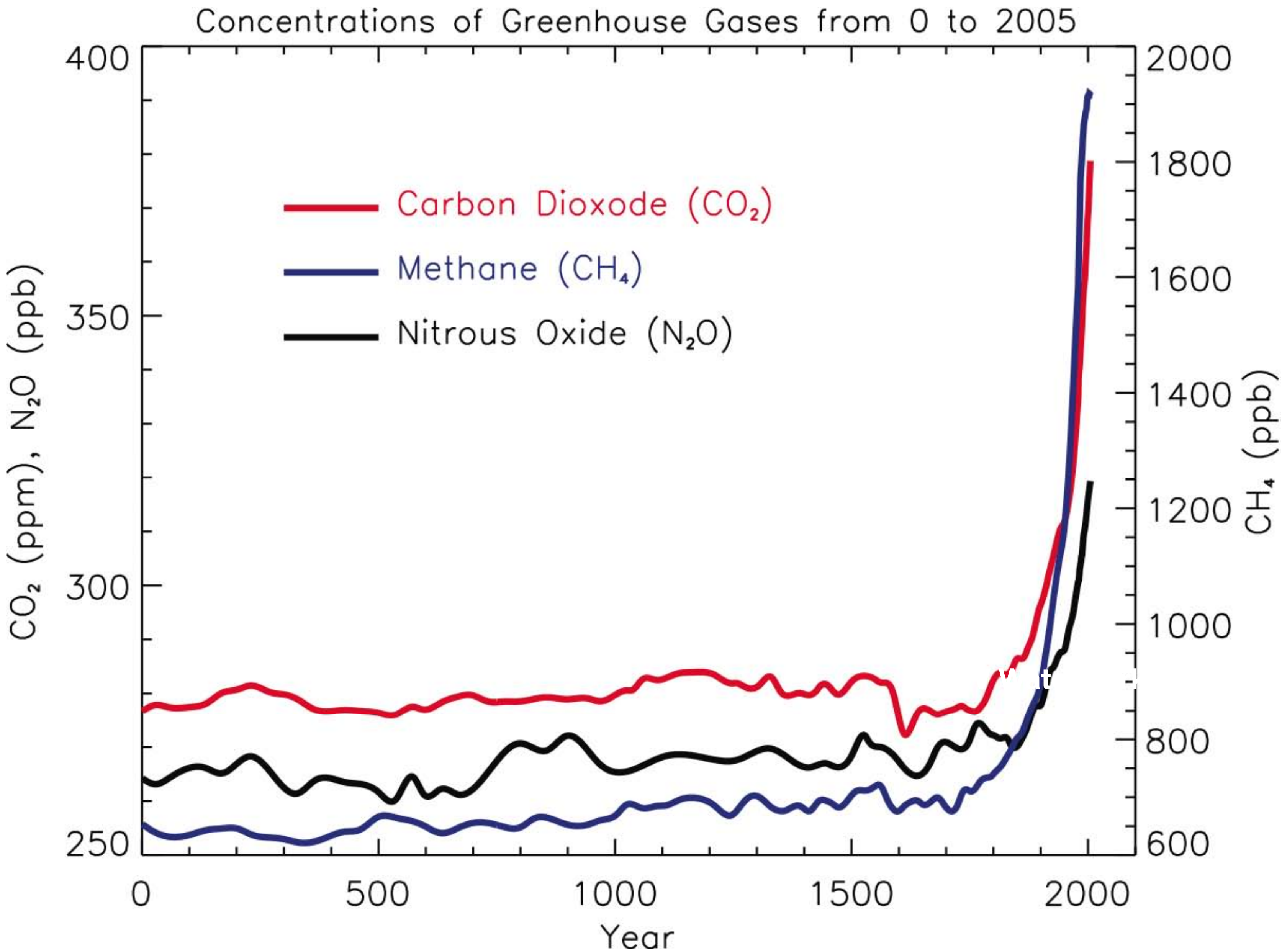
Developing World - Future in the Balance



source: gapminder.org

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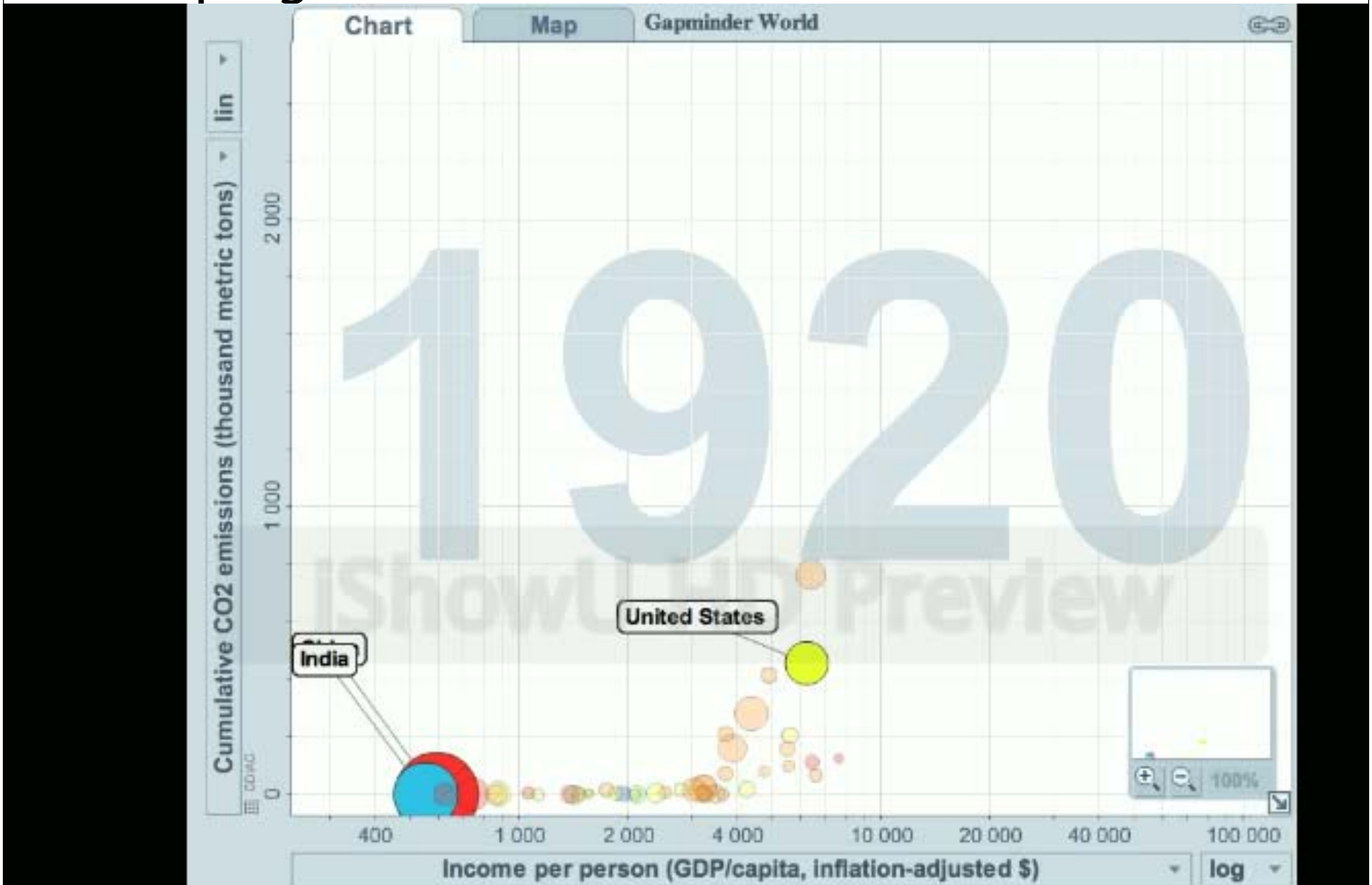

source: gapminder.org

October 22, 2011

January 04, 2012

Humanities Researchers Dig for Data

Datanami Staff

We often hear about the advantages of mining massive data sets for the benefit of big business and scientific research, but this week scholars in the humanities demonstrated their ability to find new ways to extract value from a range of data repositories.

The impetus behind the drive to encourage growth of new data processing and management tools in the humanities was spurred by a competition among academic institutions called the "Digging into Data Challenge."

Fourteen teams from the Netherlands, Canada, the UK and the US have been awarded a combined total of $4.8 million in grant funding to find ways to apply computational techniques to big data to change the nature of humanities and social sciences research.

The aims of the challenge, which started in 2009, revolve around how to address the problems of big data, which is reshaping the landscape for humanities and social sciences research. As the organizers claim, the world is becoming digitized—including the materials that researchers in the humanities and social sciences have been using for many decades (newspapers, books, etc.). This challenge is meant to spur the "research community to help create the new research infrastructure for 21st century scholarship."

stagnant. He says that too often doctors writ
unanalyzed in a system, taking up storage s

January 24, 2012

Startup Tackles University Genomics Bottlenecks

Datanami Staff

Just over a week ago we pointed to a small St. Louis-based analytics company serving the life sciences, financial services and intelligence markets called **Appistry**. At the time, they released a news item citing positive growth in their own business, while making a few notable predictions about the years to come.

Today they landed in the news again, this time due to their partnership with the nearby University of Missouri—home of a genomics research hub in the Midwest, the U of M Bioinformatics Consortium.

The University of Missouri will leverage Appistry's **life science platform** to boost their ability to handle the I/O and big data demands of plant and animal genomics research. The team will deploy the Ayrris/BIO high-performance computing platform to increase the computational scale of their automated sequencing pipelines and alleviate their data management burden.

As Appistry describes it, Arryis/BIO provides a "high-level application environment that transforms traditional analytic applications into high-performing, distributed applications for NGS. Built around a robust pipeline automation system, Ayrris / BIO shifts the responsibility for data manipulation and management from the researcher to an automated system built for massively parallel execution."

This sounds like an ideal fit for the university's genomics research program, which according to a **statement** today had hit a storage wall and was in desperate need of a data management system. The team will take advantage of the company's Computational Storage technology in hopes of eliminating bottlenecks and addressing workload management issues at scale.

AUSTRALIAN LifeScientist

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$1000 genome might be just around the corner

A new genome sequencing technology demonstrated by Oxford Nanopore could see an entire genome sequenced in under an hour by 2013.

Tim Dean (Australian Life Scientist) | 20 February, 2012 13:0

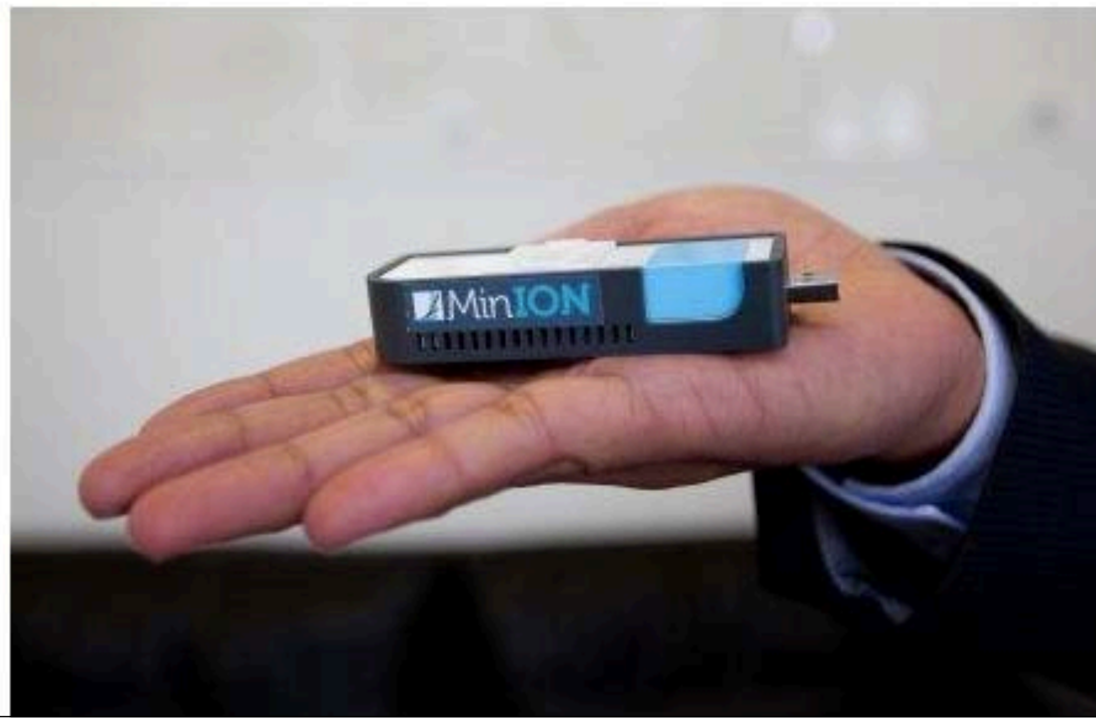
| Like 4

20 February, 2012

Share

Related Coverage

- Gene patents challenged in court
- Genetic Technologies gains access to full US market for BREVAGen
- Feature: How next generation sequencing could save the Tasmanian devil
- Genome map sheds light on deadly Tasmanian devil tumour
- Lorne 2012: Modelling



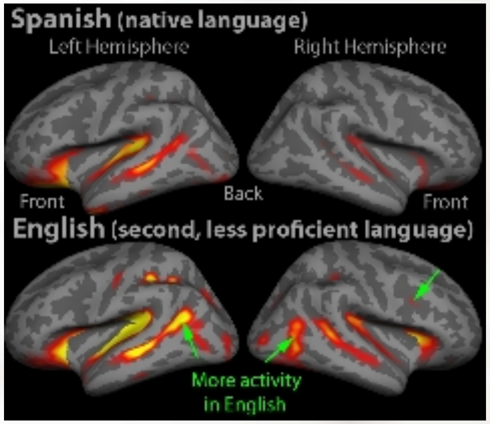
SIMULATION AND MODELING

Processes are:

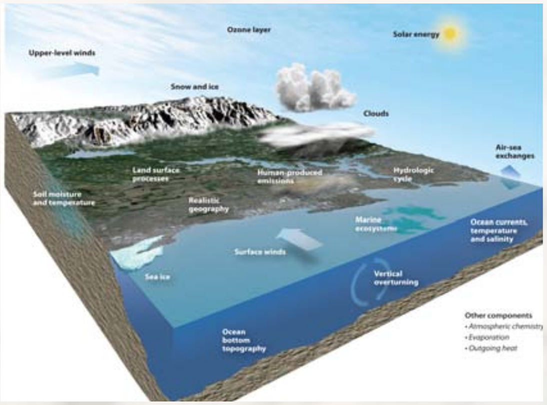
- Inherently compute intensive
- Must be repeated (Monte Carlo) to remove "noise"
- Comparisons of models
- A hardware/software issue: Not all problems can be subdivided and distributed but must be run in parallel

Applications in:

- Decision making and global climate change
- Brain function and specialization
- Learning



Credit: Matthew K Leonard, University of California, San Diego

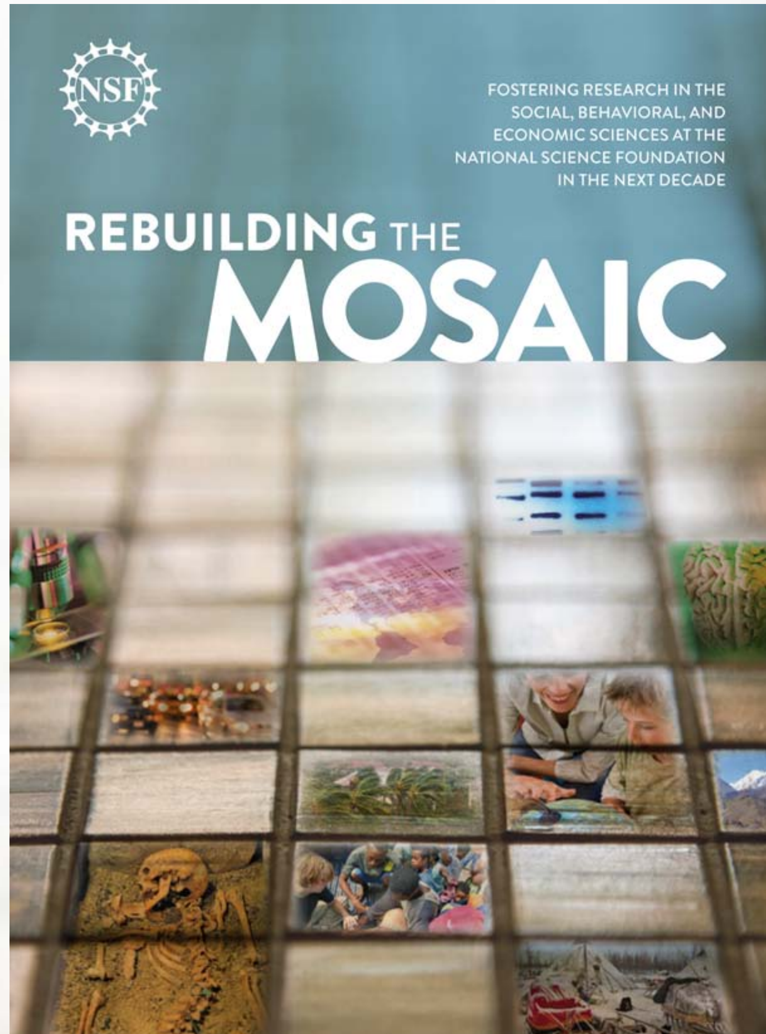


Avian Flu Timeseries

www.nature.com

FUTURE SBE RESEARCH: TECHNOLOGY AND DATA DRIVERS

- Scale: More data from more sources (environmental, sensor, administrative, survey, commercial, usage, and so on)
- Density (merge, overlap, georectify)
- Tools (statistics, GIS, network analysis, modeling, scenarios)
- Granularity (fMRI, administrative, commercial and behavioral level)
- Greater access to and demand for high performance computational resources



Slide courtesy of Myron Gutmann, Directorate for Social, Behavioral and Economic Sciences, March 2012

The New York Times Technology | Personal Tech | Business Day

Bits

What Are the Odds That Stats Would Be This Popular?

By QUENTIN HARDY | January 26, 2012, 10:30 AM | 1

- Statisticians are popular?
- Programs place 90% of their students with average entry salaries of $73,000
- New jobs with “analytics” grew by 53% from 2009-2011
- Applications at Google, Facebook, risk analysts, spies, natural philosophers, gamblers.

Top 15 Jobs in 2011 (Wall St Journal)

	Title	Mid-level Income
1	software engineer	$87,000
2	mathematician	$94,000
3	actuary	$87,000
4	statistician	$73,000
5	computer systems analyst	$77,000
6	meteorologist	$85,000
7	biologist	$74,000
8	historian	$63,000
9	audiologist	$63,000
10	dental hygienist	$67,000
11	sociologist	$70,000
12	accountant	$60,000
13	paralegal assistant	$47,000
13	physicist	$106,000
15	financial planner	$101,000

http://online.wsj.com/public/resources/documents/st_BESTJOBS0104_20110105.html

SUMMARY

- Many challenges facing the nation and the world
- Math and computers can help solve society's problems
- Data analysis will become an important component in all areas
- We need many more people working on these problems

SO IF SOMEONE ASKS YOU WHY YOU'RE STUDYING MATH?

I'm Going To Help Save The World!


TRASH