The Role of Mathematics in Amplifying Science Research

How Mathematics Will Help Save The World

Juan Meza

Lawrence Berkeley National Laboratory

Northern California Undergraduate Mathematics Conference

Sonoma State University, April 19, 2008

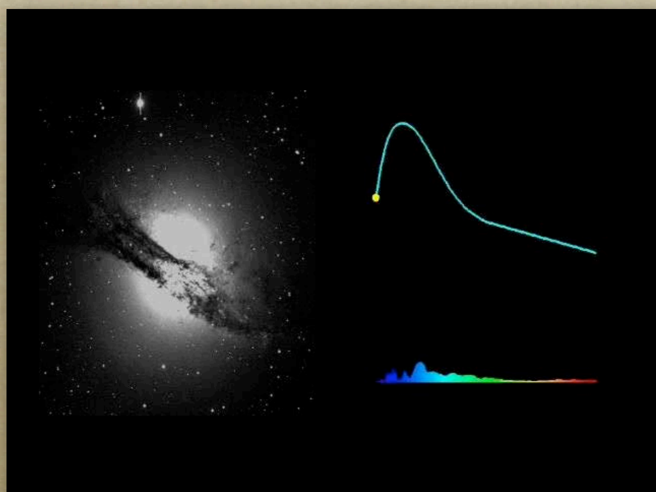
Amplifying the advancement of science and engineering research

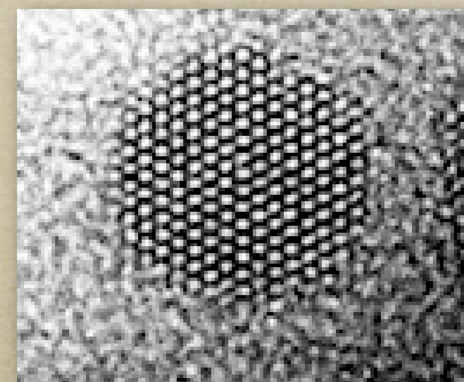
*Previously, research was **experimental, observational or analytical**. Progress in computer and information science and engineering not only advances information technology itself, but leverages advancement of knowledge in other areas.*

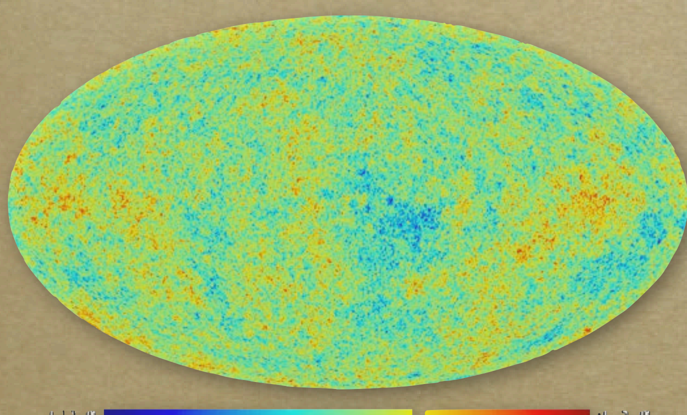
It shares this trait with mathematics. ...., *by amplifying the efficiency and productivity of almost all other areas of our economy as well as **amplifying the advancement of science and engineering research.***

Anita Jones
Quarles Professor of Engineering & Applied Science, University of Virginia
Before the Subcommittee on Research, House Committee on Science, June 16, 2001

Broader use of computational math and sciences for scientific discovery







Climate Change is Big News

THE TIMES

Nation & World

MONDAY, MARCH 24, 2008 For more reports: ContraCostaTimes.com SVE PAGE

Forecasters warn of historic floods in Arkansas

By Jon Gambrell

Robinson wrote in an e-mail to reporters Sunday.

A tributary of the White River, the Black River, ruptured a levee in two places Saturday near Pocahontas, said Renee Preslar, a spokeswoman for the Ar… Department of Emergenc… agement.

That stream has been … by water pouring down… from hard-hit southeaster… souri.

Preslar said the levee … allowed flooding in outly… eas but she did not have … on what might have bee… aged.

The Army Corps of En…

worked through the night to plug the breaks with sandbags, and that work appeared to be holding as of Sunday afternoon, Preslar said.

"Right now, it's kind of a wait-…

time, they had closure gates on them, but they couldn't be closed" Saturday, Spaul said. "Everything was rusted out on them."

Arkansas emergency man-…

Last week's torrential rainstorms also caused flooding in parts of Ohio and southern Illinois and in wide areas of Missouri.

At least 17 deaths have been …

8 For more reports: ContraCostaTimes.com

ANTARCTIC ICE SHELF COLLAPSES

NASA

THIS SATELLITE PHOTO shows the Wilkins Ice Shelf beginning to break apart March 6. Part of the ice shelf suddenly collapsed, scientists said Tuesday. Experts blame global warming for the disintegration.

Glacial melt worries scientists

By Seth Borenstein
ASSOCIATED PRESS

WASHINGTON — A chunk of Antarctic ice about seven times the size of Manhattan suddenly …

ONLINE
- The National Snow and Ice Data Center: http://nsidc.org
- The British Antarctic Survey: …

There's still a chance the rest of the ice shelf will survive until next year because this is the end of the Antarctic summer and colder weather is setting in, …

PLEASANTON • LIVERMORE • DUBLIN

THE VALLEY TIMES

Edition of the Contra Costa Times

Tuesday, March 25, 2008 ContraCostaTimes.com Volume 96, Number 299 50 cents plus tax

Future of Lake Tahoe looks murky, study says

■ UC Davis researchers predict climate change will cause permanent damage

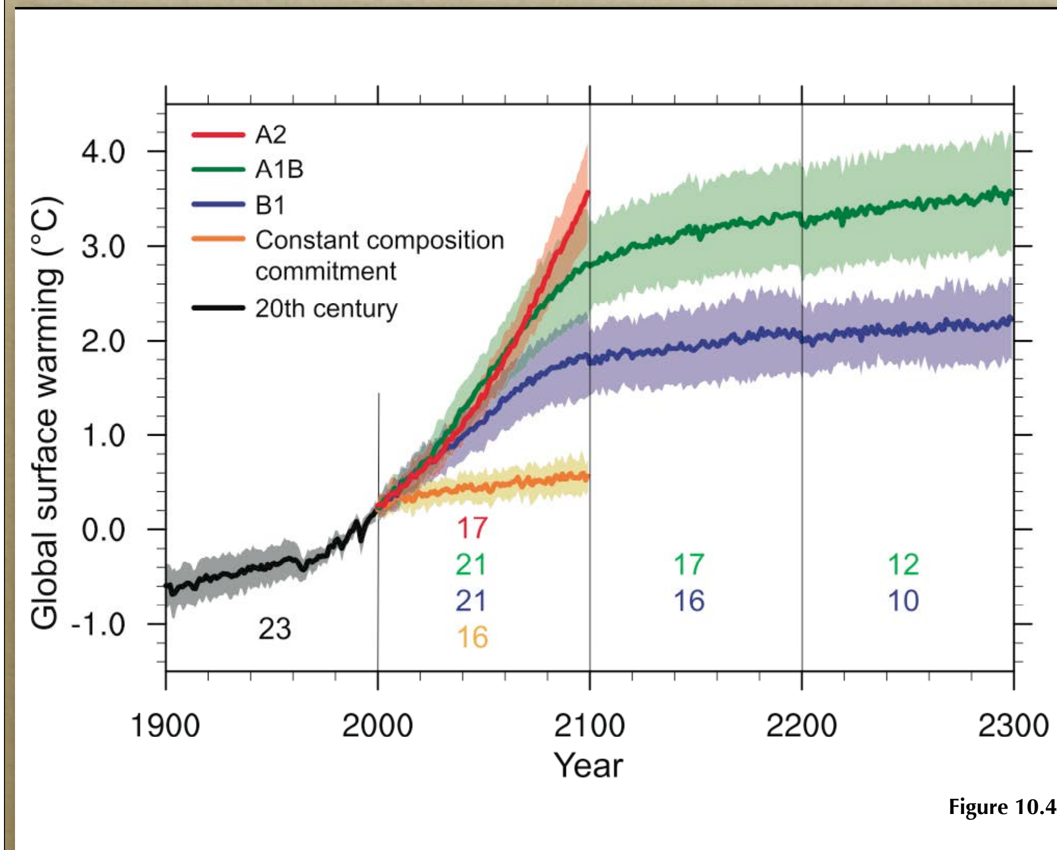
By Julie Sevrens Lyons
MEDIANEWS STAFF

The jewel of the Sierra could be worse off than previously thought.

Global warming already is causing warmer lake temperatures along the shoreline, and it is likely to continue to cloud up the cobalt waters that attract tourists from all over the world. However, the most recent news came as a shock to even the researchers.

"This is one of the early indi-

We'll consider three areas where math is being used to study effects of climate change



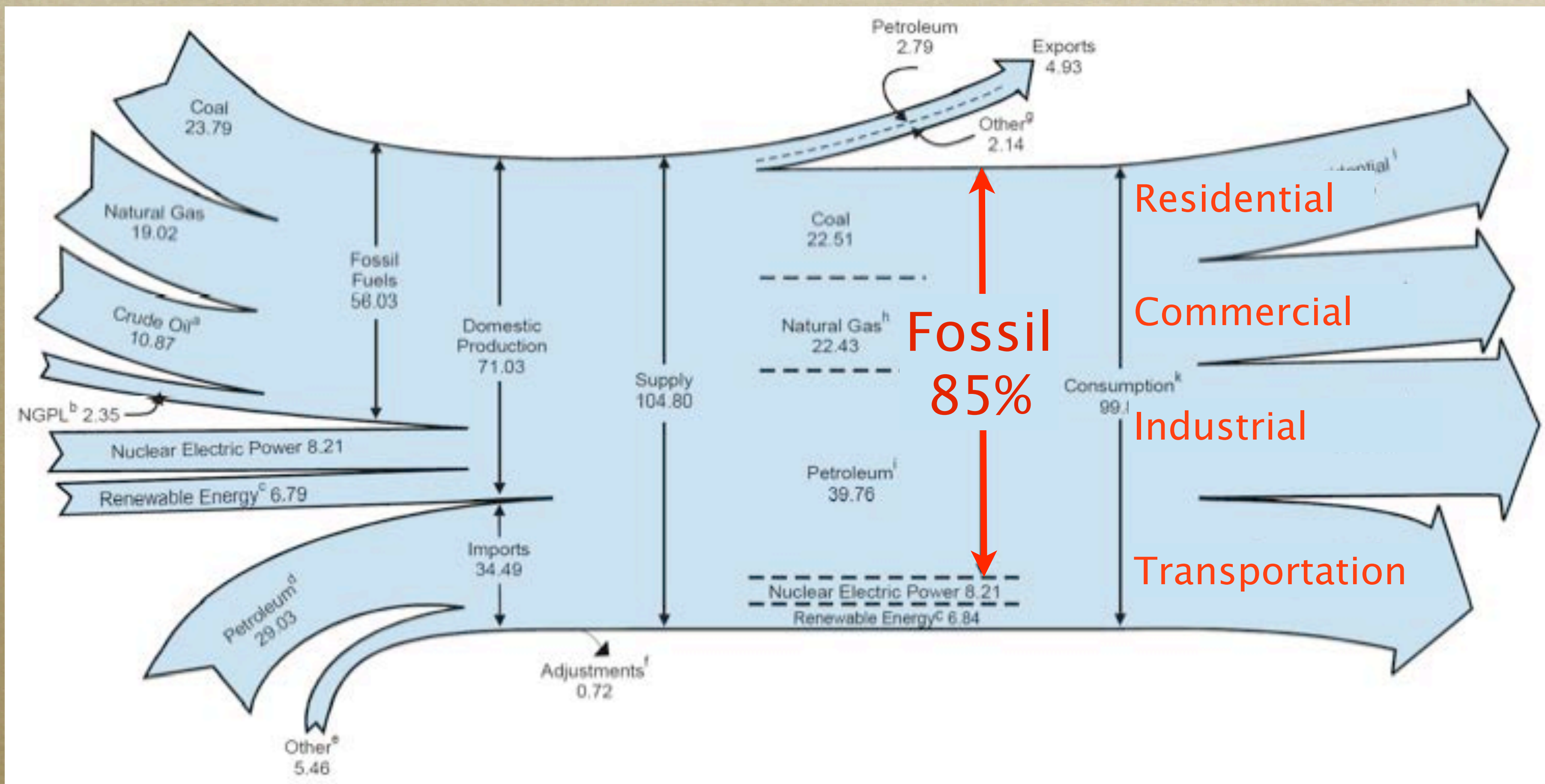
http://ipcc-wg1.ucar.edu/wg1/wg1_home.html

- ***What are we doing today to improve our use of energy?***
- ***What can we do to change how we use energy in the future?***
- ***What can we say about our future climate and its effects on us?***

Energy Today

85% of our energy comes from fossil fuels

US Energy Flow in 2006 was 100 Quads

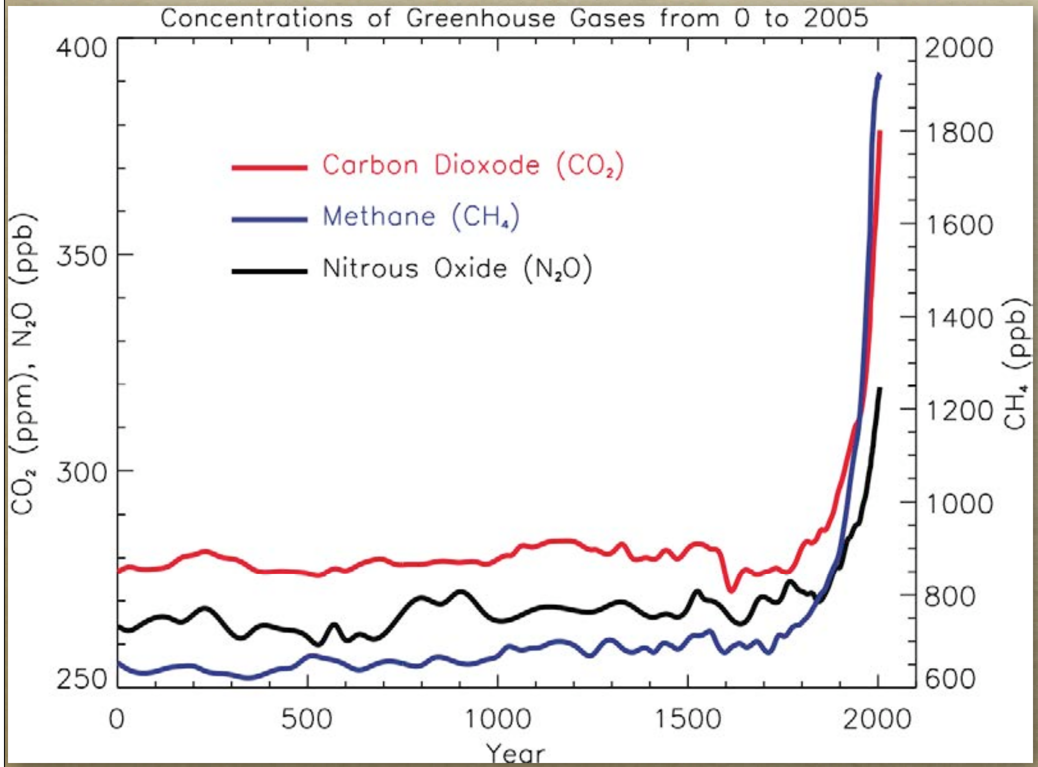


Annual Energy Review, Energy Information Administration, http://www.eia.doe.gov/aer/

Combustion of fossil fuels accounts for 85% of our energy

- *Combustion*
    - *Transportation*
    - *Power generation*
- *Particulates are potential sources of health problems*
- *Exhaust gases are a primary source of anthropogenic greenhouse gases*

Annual global release of CO_2 is 27 Billion Tons

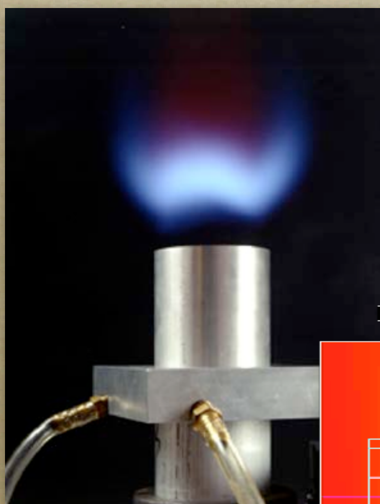


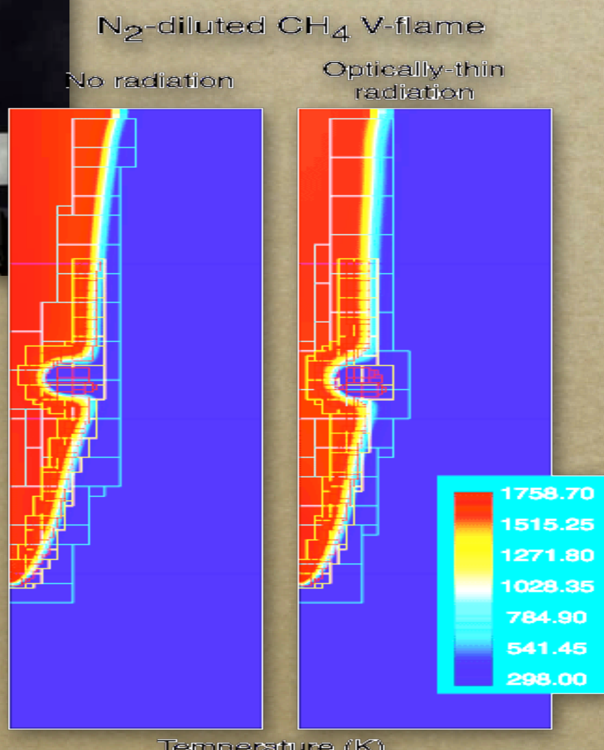
- ***40% coal, 40% oil, 20% natural gas***
- ***US consumes (per day):***
  - ***20 million barrels of oil***
  - ***60 billion cubic feet natural gas***
  - ***3 million tons of coal***

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

Increasing combustion efficiency is important in reducing greenhouse gases

Low Swirl Burner

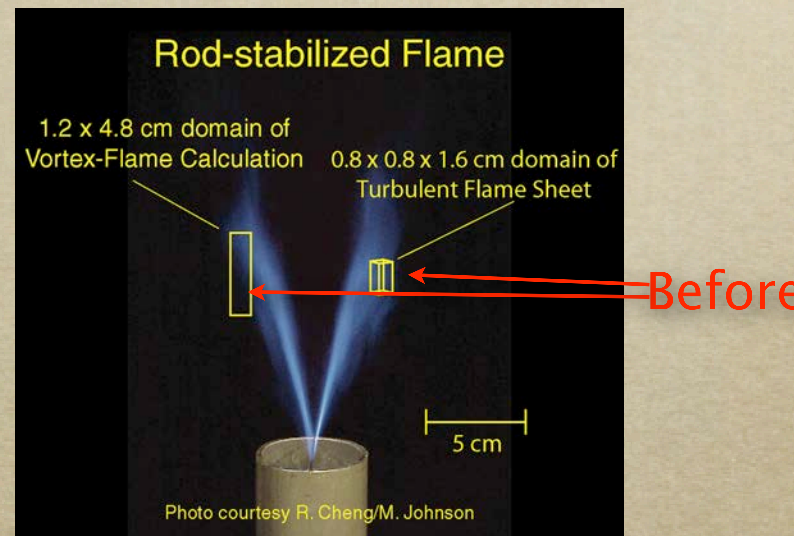




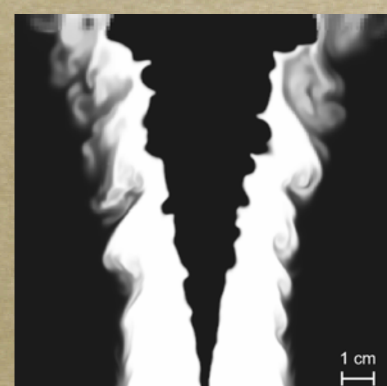
- *Most new systems are based on lean premixed turbulent combustion*
- *Lean premixed systems have potentially high-efficiency and low emissions*
- *Challenges to system design*
  - *Natural flame instabilities*
  - *Sensitivity to fuel*

Mathematics group increased simulation capability by a factor of 10,000

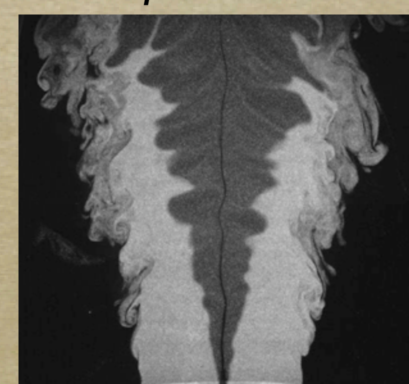
- *Advances in applied mathematics have dramatically increased our simulation capability*
- *Mathematical formulation to exploit separation of scales*
- *Specialized discretization methods*
- *Adaptive mesh refinement*
- *Parallel numerical algorithms*



Simulation



Experiment

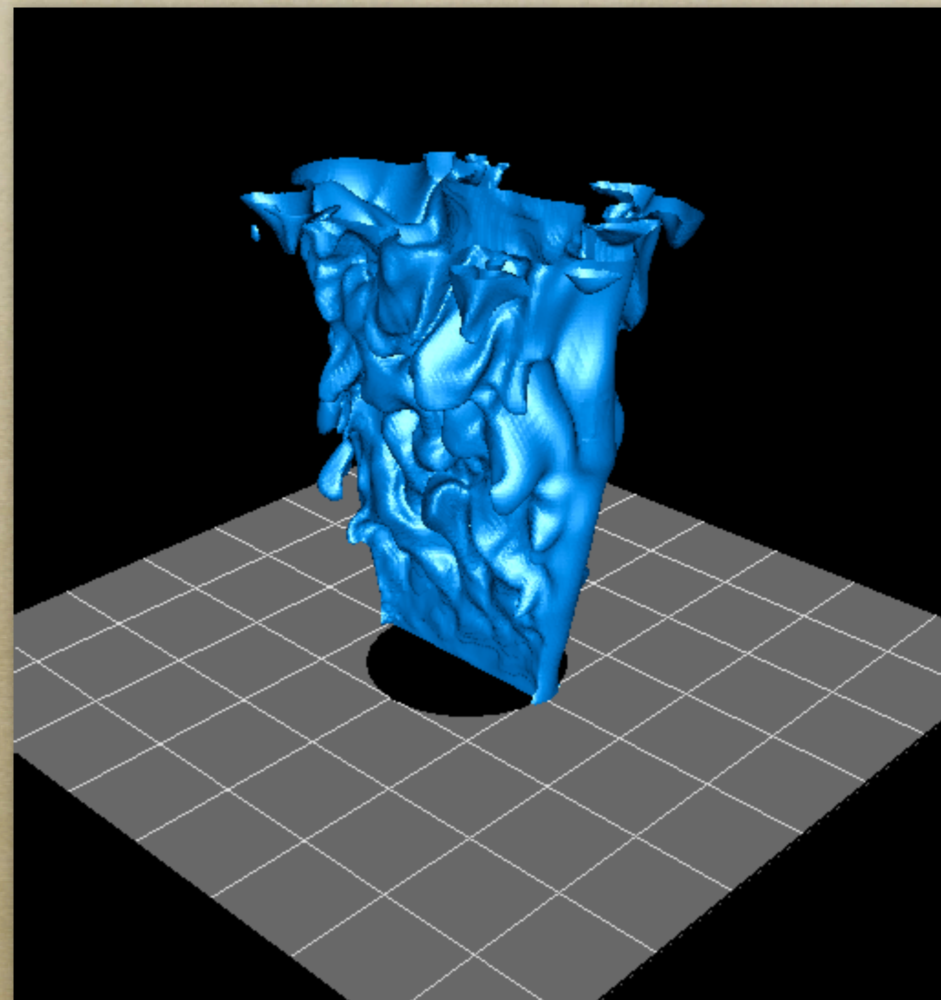


Turbulent Premixed V-Flame

Experimental Turbulent V-Flame

(photo courtesy R. K. Cheng, LBNL)

Calculations



Low Mach number equations

$$\begin{aligned}
\rho \frac{DU}{Dt} &= -\nabla \pi + \nabla \cdot \tau \quad \text{Momentum} \\
\frac{\partial \rho Y_m}{\partial t} + \nabla \cdot (\rho U Y_m) &= \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m \quad \text{Species} \\
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) &= 0 \quad Mass \\
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h U) &= \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m) \quad Energy
\end{aligned}$$

Y_m mass fraction

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

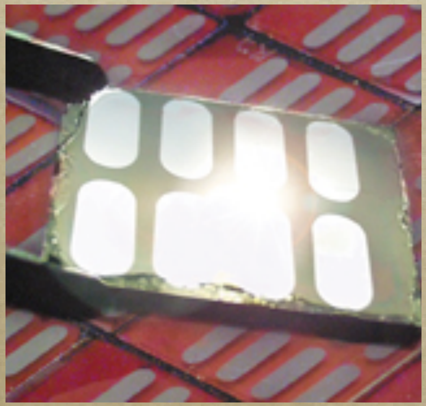
h enthalpy, $h = \sum Y_m h_m(T)$

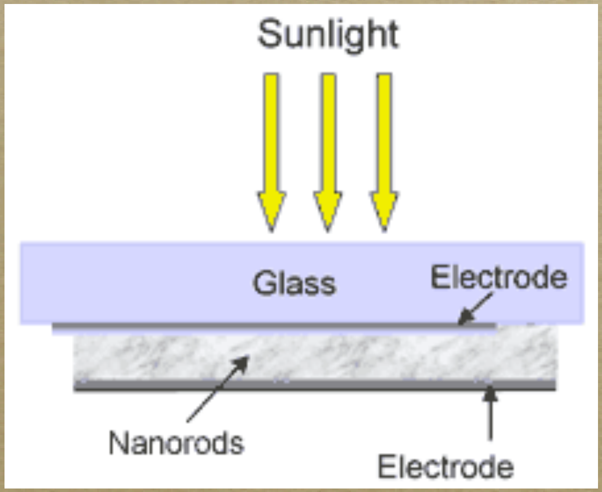
Equation of State $p_0 = \rho R T \sum Y_m / W_m$

Energy Tomorrow

More energy from sunlight strikes the Earth in one hour than all the energy consumed on the planet in a year

Photovoltaic Solar Cells

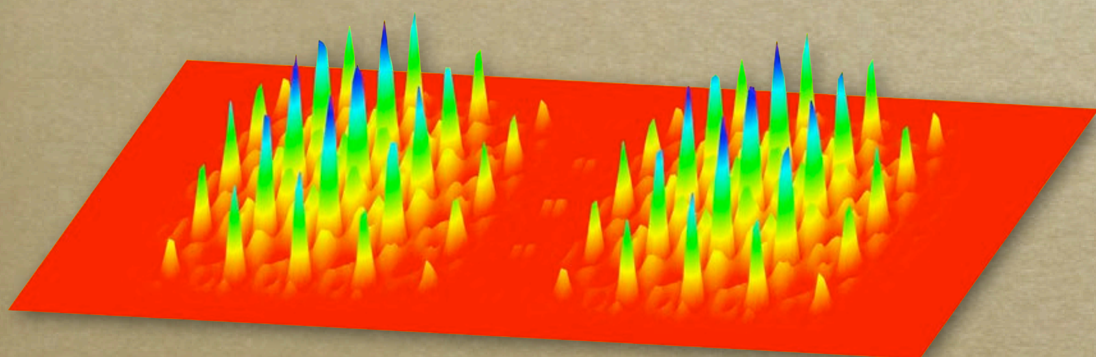




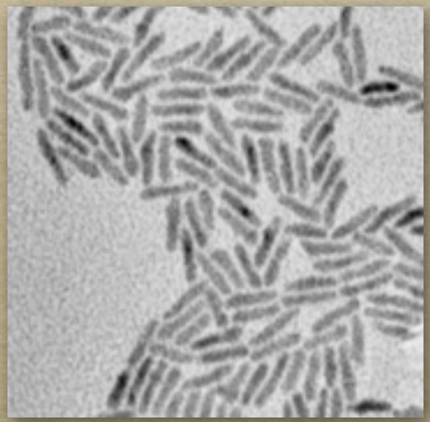
- *Solar cells based on inorganic nanorods and semiconducting polymers*
- *Nanorods can be made of CdSe, a semiconducting material*
- *Nanorods act like wires, absorbing light and generating hole-electron pairs*
- *Biggest challenge is cost, ~30 cents/kWh*

Computational Nanoscience

- *The electronic structure and optical properties change with the shape of the quantum rods*
- *Thousand atom quantum rods can be simulated using a planewave density functional theory method*
- *But current methods are computationally expensive*



The electron wavefunctions of quantum rods

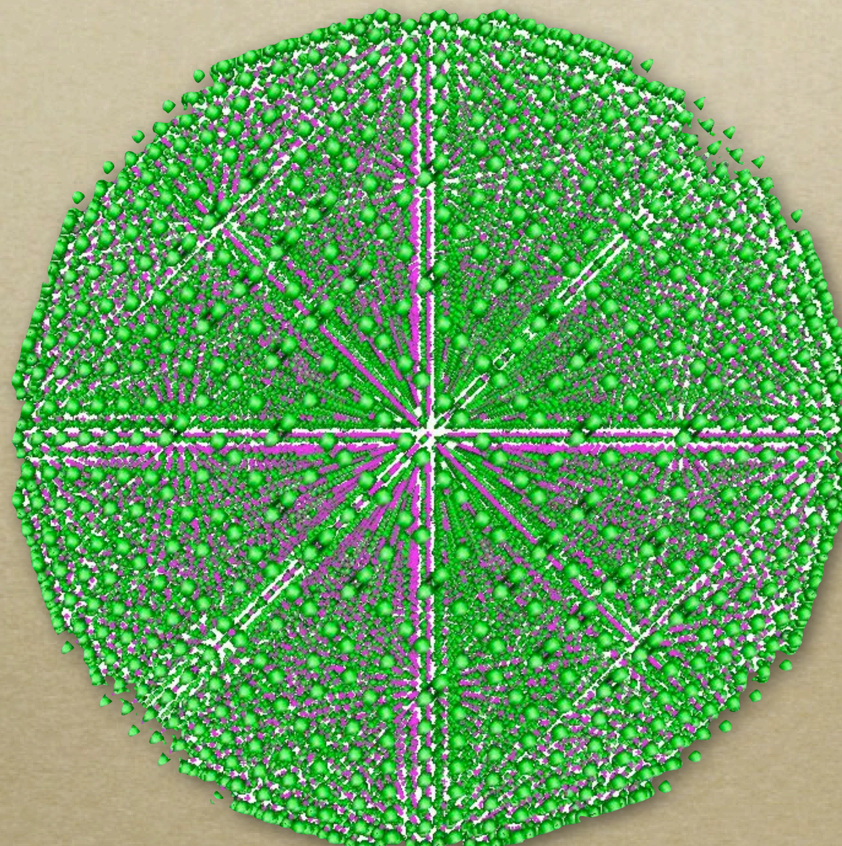


CdSe quantum rods

Andrew Canning, Lin-Wang Wang, Scientific Computing, LBNL

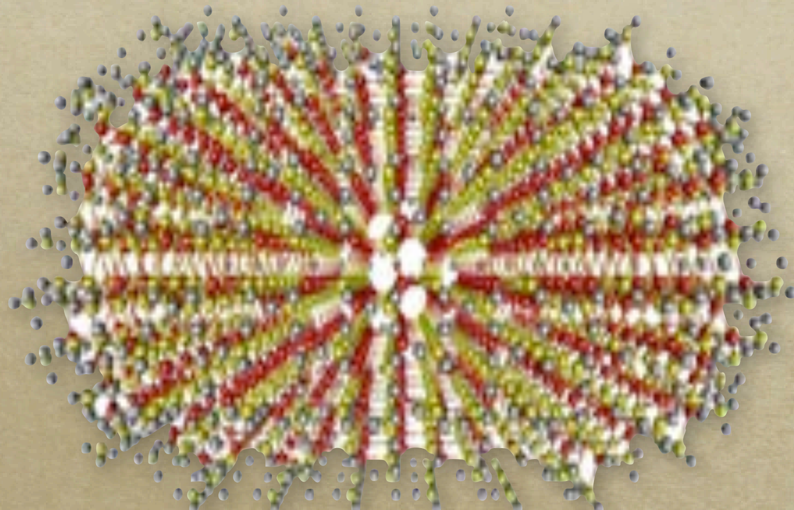
New Linearly Scaling Method Decreases Computational Time by a Factor of 400

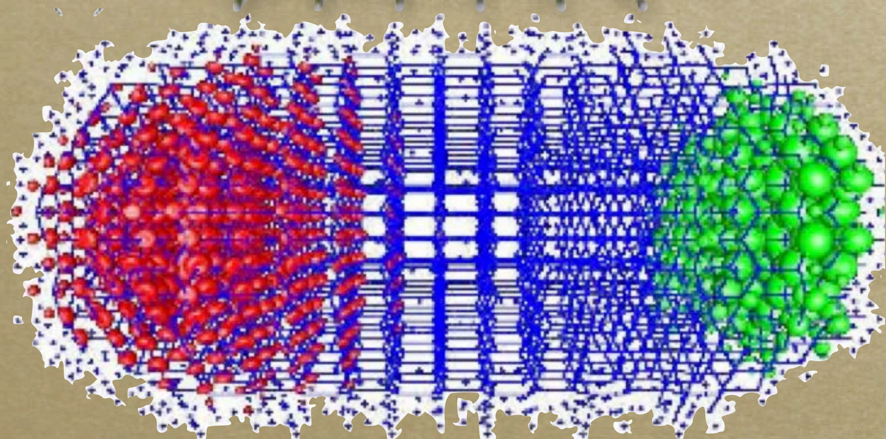
- *The charge density of a 15,000 atom quantum dot, $Si_{13607}H_{2236}$.*
- *A direct LDA calculation would have taken a few months.*
- *Using 2048 processors at NERSC and new algorithms the calculation takes about 5 hours*



A divide-and-conquer linear scaling three dimensional fragment method for large scale electronic structure calculations, Wang, Zhao, Meza, in press

Dipole Moment Calculations Help to Explain Experiments





- *Experiments show that these structures have a dipole moment*
- *The calculated dipole moment of a 2633 atom CdSe quantum rod, $Cd_{961}Se_{724}H_{948}$*
- *Using 2560 processors at NERSC the calculation took about 30 hours.*

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

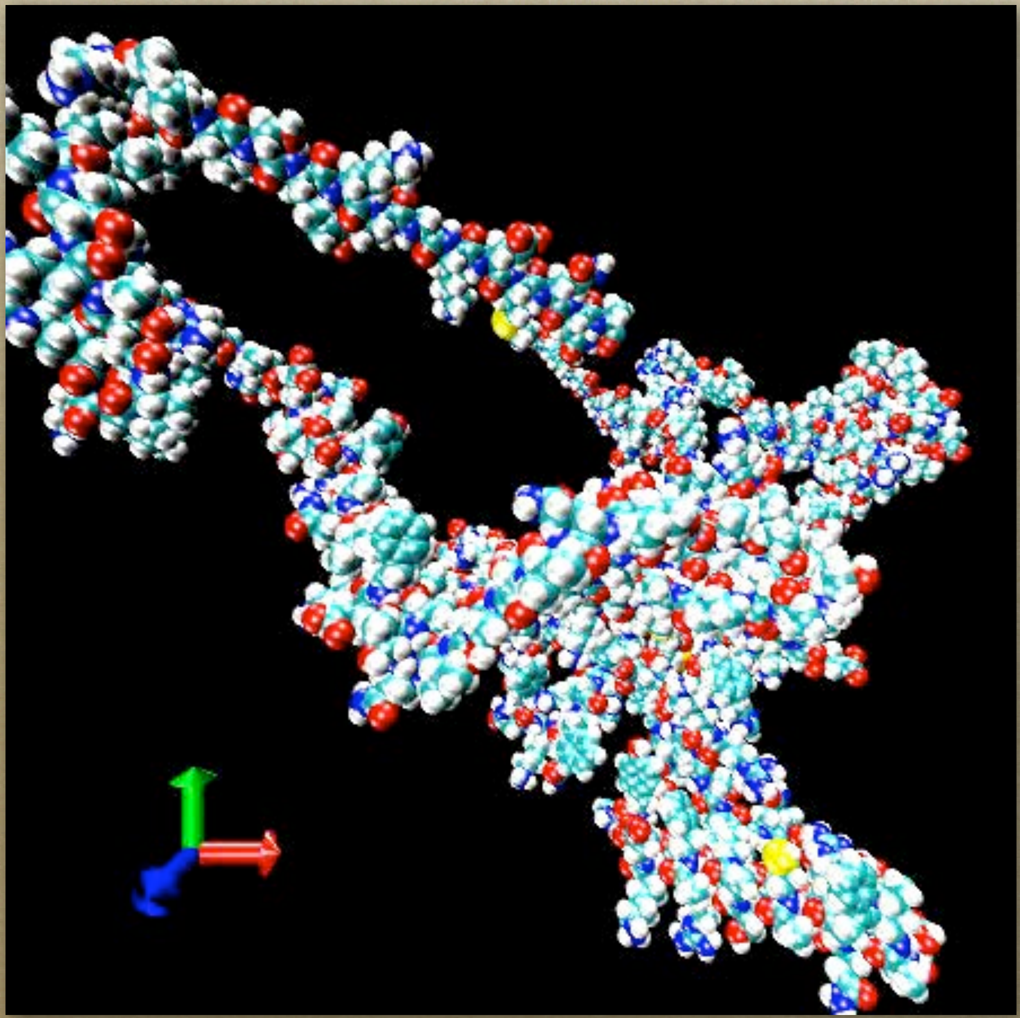
Density functional theory and the Kohn-Sham equations

$$E_{total}[\{\psi_i\}] = \frac{1}{2}\sum_{i=1}^{n_e}\int_\Omega |\nabla\psi_i|^2 + \int_\Omega V_{ext}\rho + \frac{1}{2}\int_\Omega \frac{\rho(r)\rho(r')}{|r-r'|}drdr' + E_{xc}(\rho),$$

$$\rho = \sum_{i=1}^{n_e} |\psi_i(r)|^2, \int_\Omega \psi_i\psi_j = \delta_{i,j}$$

$$\left[-\frac{1}{2}\nabla^2 + V_{ext}(r) + \int \frac{\rho}{|r-r'|} + V_{xc}(\rho)\right]\psi_i = \epsilon_i\psi_i$$

Bio-molecules also hold promise



- *Energy minimization computed using a large-scale optimization method*
- *Solution matched experimental data to within 3.9 Å*
- *Total simulation took approximately 32 hours on a workstation*

Juan Meza, Ricardo Oliva, Scientific Computing, LBNL

Amber Force Field Equations

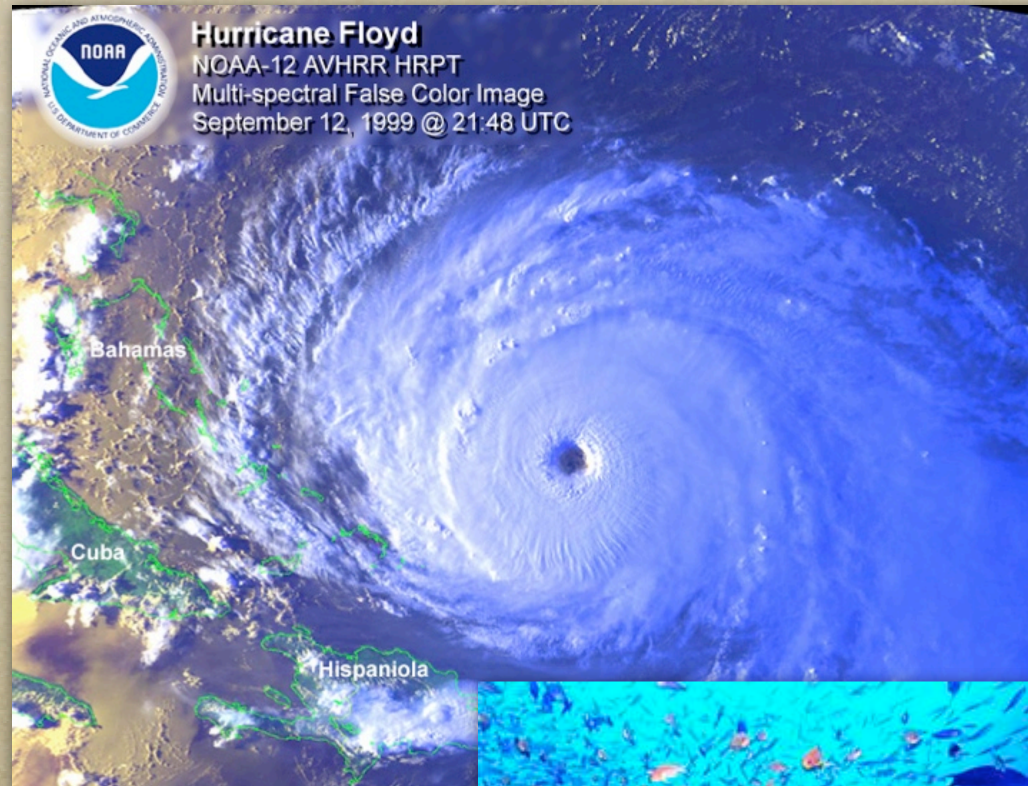
$$
\begin{aligned}
E_{total} &= E_{bond} + E_{angle} + E_{dihedral} + E_{nonbond} \\
E_{bond} &= \sum K_b (r_i - \bar{r_i})^2 \\
E_{angle} &= \sum K_\theta (\theta_i - \bar{\theta}_i)^2 \\
E_{dihedral} &= \sum K_\phi (1 + cos(n_i \phi_i - \delta_i)) \\
E_{nonbond} &= \sum_i \sum_{i<j} \left[\epsilon_{ij} \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{\epsilon_0 r_{ij}}
\end{aligned}
$$

A Physical Approach to Protein Structure Prediction, Crivelli, et.al. Biophysical Journal, Vol 82, 2002.

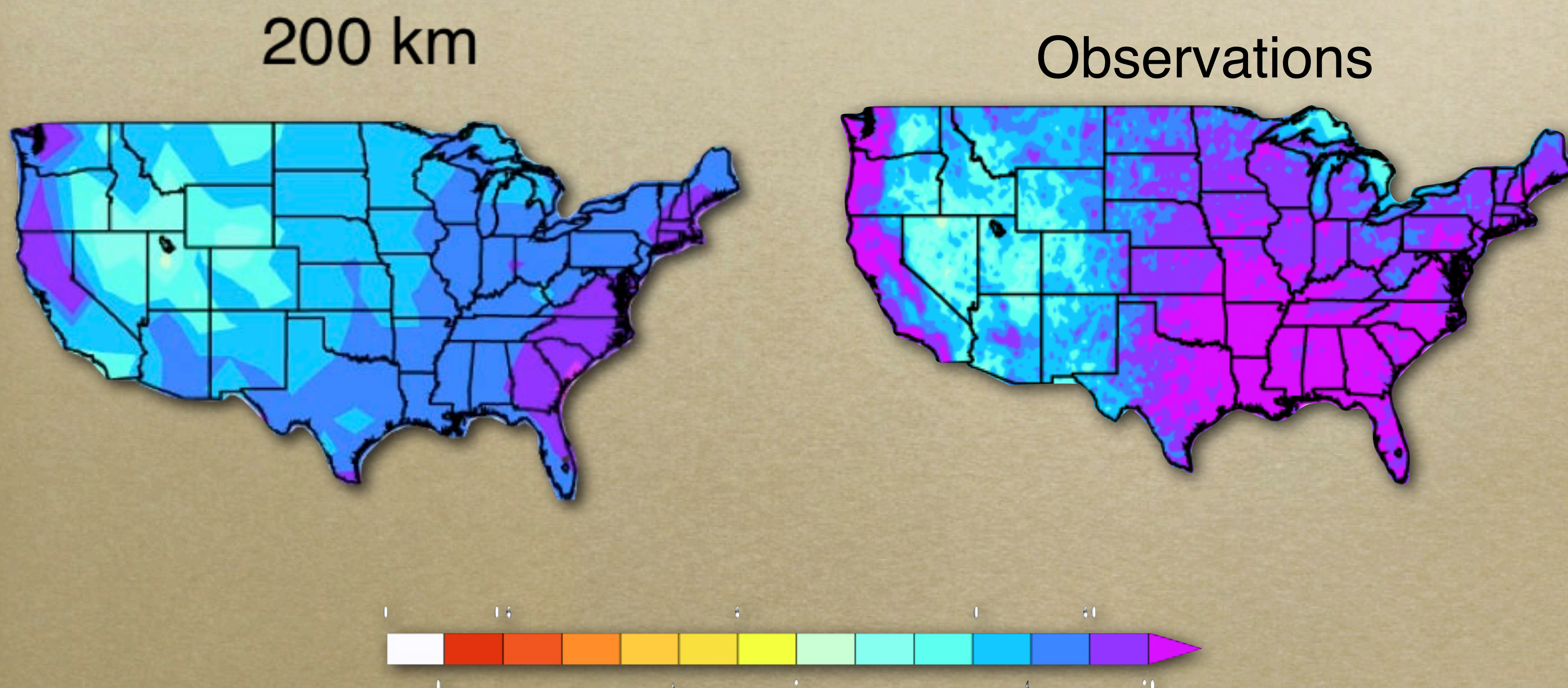
Consequences

The major difference between a thing that might go wrong and a thing that cannot possibly go wrong is that when a thing that cannot possibly go wrong goes wrong it usually turns out to be impossible to get at or repair

Douglas Adams

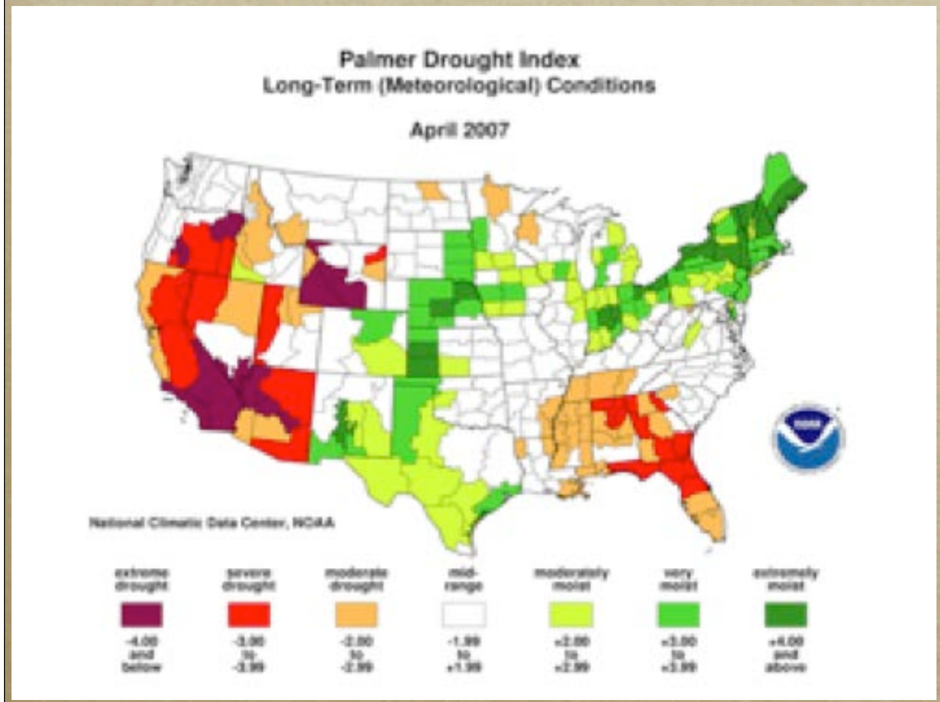

Hurricane Floyd
NOAA-12 AVHRR HRPT
Multi-spectral False Color Image
September 12, 1999 @ 21:48 UTC
Bahamas
Cuba
Hispaniola

Extreme precipitation as a function of horizontal resolution



*20 year annual maximum daily precipitation return value (M.F. Wehner (LBNL) et al. work in progress)

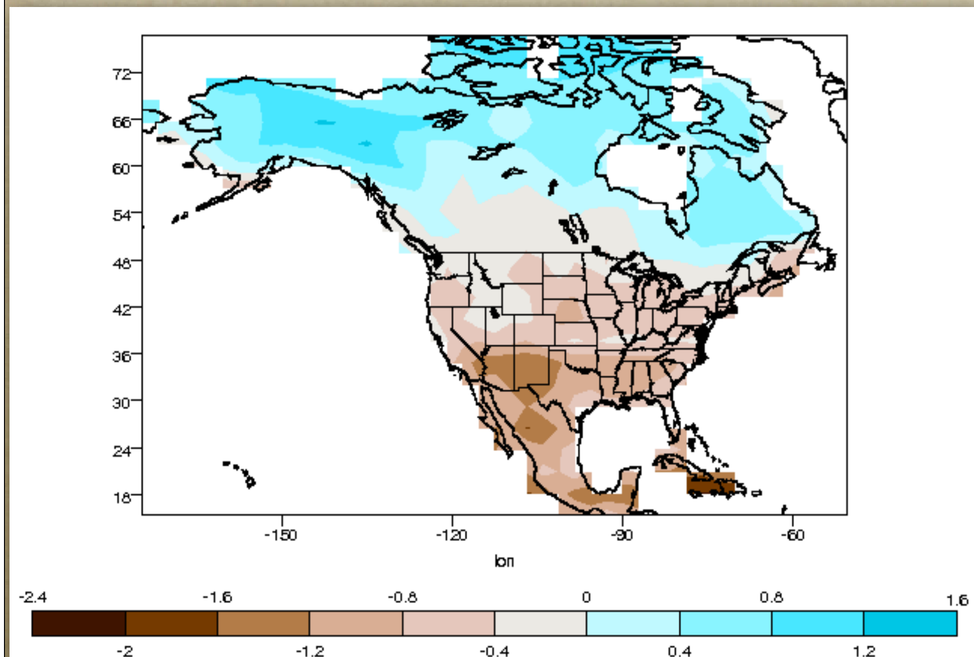
Palmer Drought Index



- *The Palmer Drought Index (PDI) maps show long-term (cumulative) meteorological drought and wet conditions.*
- *The maps show how the geographical pattern of the long-term moisture conditions has changed over the last 12 months.*
- *The red shading denotes drought conditions while the green shading indicates wet conditions.*

http://lwf.ncdc.noaa.gov/oa/climate/research/prelim/drought/pdiimage.html

Drought conditions increase in SW US and Mexico



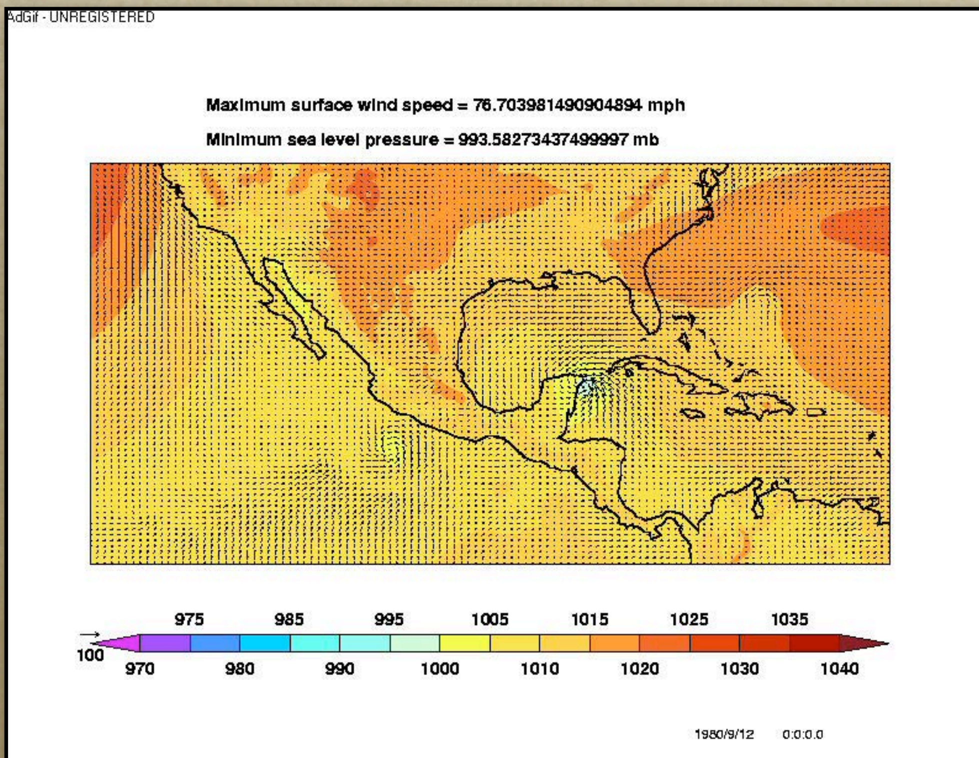
Drought ⟷ *Flood*

The predicted average value of PDSI in 2090 using the 1950-1999 period as a reference. Analysis of 22 models contributed to IPCC AR4 database

M.F. Wehner (LBNL) et al. work in progress

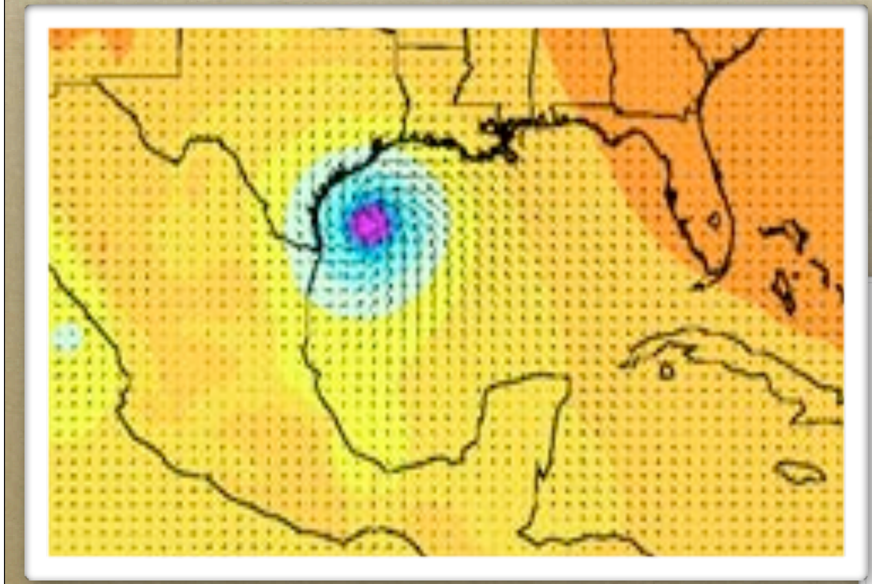
- *Most of SW US and Mexico would be in drought, while most of Canada would be in flood conditions.*
- *Precipitation decreases in the Southwest and increases substantially in the Northern latitudes.*
- *The CO2 content of the atmosphere stabilizes to 720ppm in the middle of the 22nd century.*

Climate modeling and predicting hurricane patterns

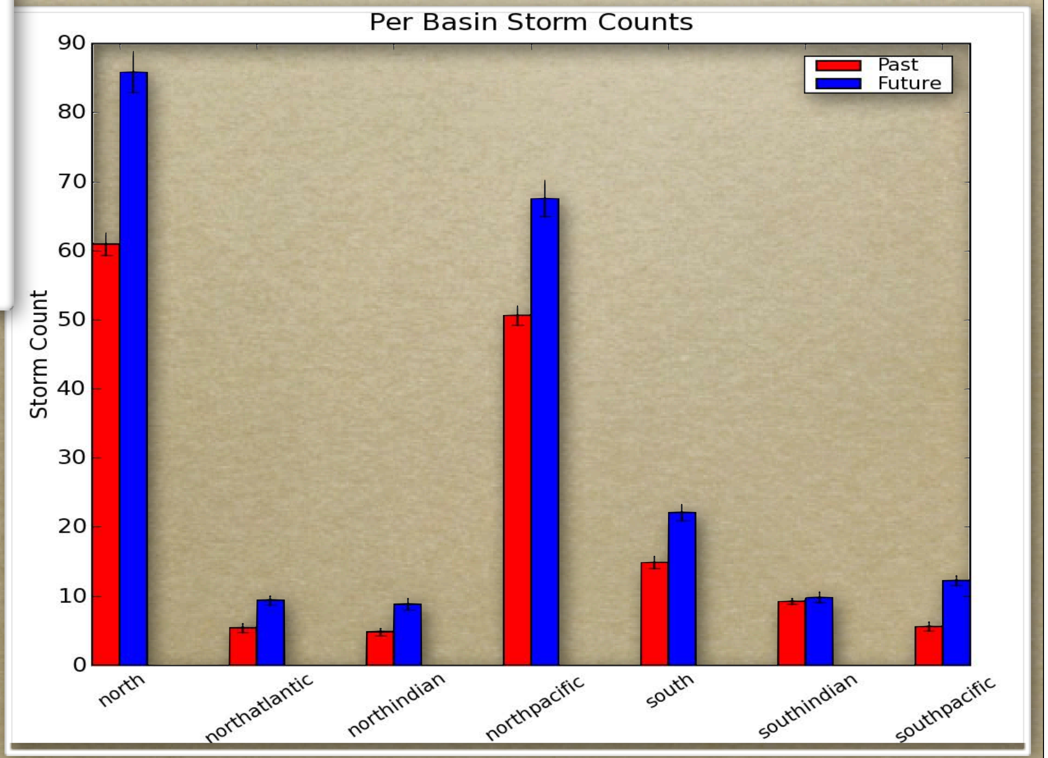


- *Tropical cyclones are not generally seen global atmospheric general circulation models at climate model resolutions T42 (~300km)*
- *In high resolution simulations of the finite volume dynamics version of CAM2, strong tropical cyclones are*

Simulated present day and end of century hurricane count



50km captures realistic tropical cyclone characteristics



The Generalized Extreme Value (GEV) distribution can be used to study climate

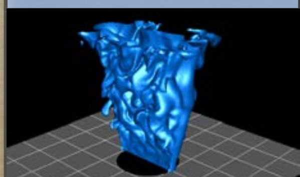
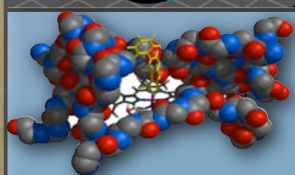
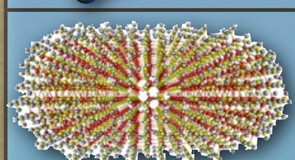
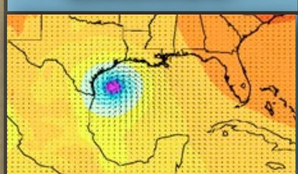
$$F(x) = \begin{cases} e^{-[1+\xi(x-\mu)/\sigma]^{-1/\xi}} & , \quad \xi \neq 0 \\ e^{-e^{-(x-\mu)/\sigma}} & , \quad \xi = 0 \end{cases}$$

$$\text{where} \quad \mu = \text{location}, \sigma = \text{scale}, \xi = \text{shape}$$

The return value of a random variable, X_T is that value that is exceeded, on average, once in a period of time, T

$$X_T = \begin{cases} \mu + \sigma[1 - \{-ln(1 - 1/T)\}^{-\xi}/\xi & , \quad \xi \neq 0 \\ \mu - \sigma[ln(-ln(1 - 1/T)) & , \quad \xi = 0 \end{cases}$$

Where did we use mathematics in these problems?

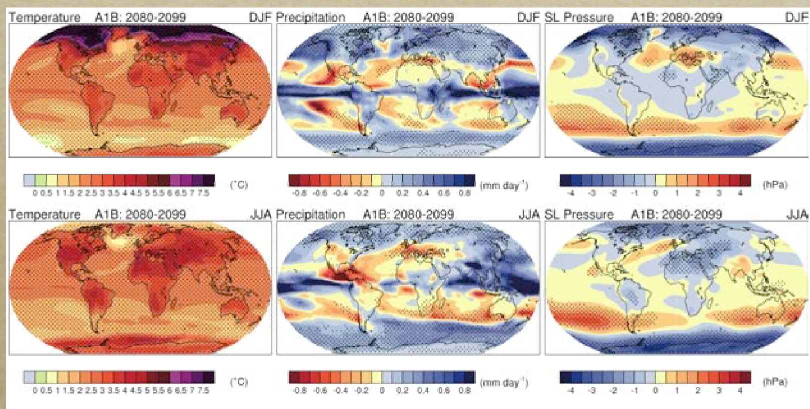
	Diff. Eq.	*Linear Algebra*	*Nonlinear Eq. & Opt.*	*Data mining / statistics*
	✓	✓	✓	✓
		✓	✓	
	✓	✓	✓	
	✓	✓	✓	✓
	Math 241	*Math 222, 322*	*Math 352*	*Math 250, 316, 365*

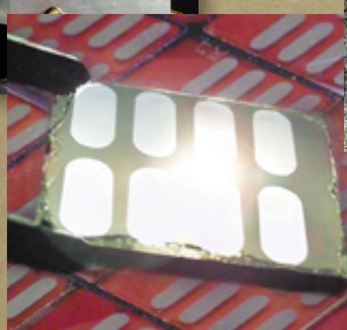
Summary

- *Computational mathematics is increasingly being used to explore science problems*
- *Many different mathematical areas are needed*
  - *Differential Equations – climate, combustion*
  - *Fast Fourier transforms – materials sciences*
  - *Linear Algebra - nanoscience, combustion,climate,bio-molecules*
  - *Nonlinear equations and optimization - everything*
  - *Statistics - climate, combustion*
- *New mathematical advances needed everyday to solve real-world problems*

Mathematics accelerates the discovery of science AND will continue to do so

Future Work





- *Understand and predict future climate scenarios*
- *Develop more efficient, environmentally friendly combustion processes*
- *Design new, more efficient materials for renewable energy: solar, biofuels, ...*

So If Someone Asks You
Why You're Studying Math?
or
What Are You Going To Do
With A Math Major?

I'm Going To Help Save
The World!

Dedicated to Rachel and Jeremy

Thank you !