

*Computational Nanoscience*  
*NSE C242 & Phys C203*  
*Spring, 2008*

**Lecture 29:**  
**Verification & Validation -- and Some**  
**Examples**  
**May 6, 2008**

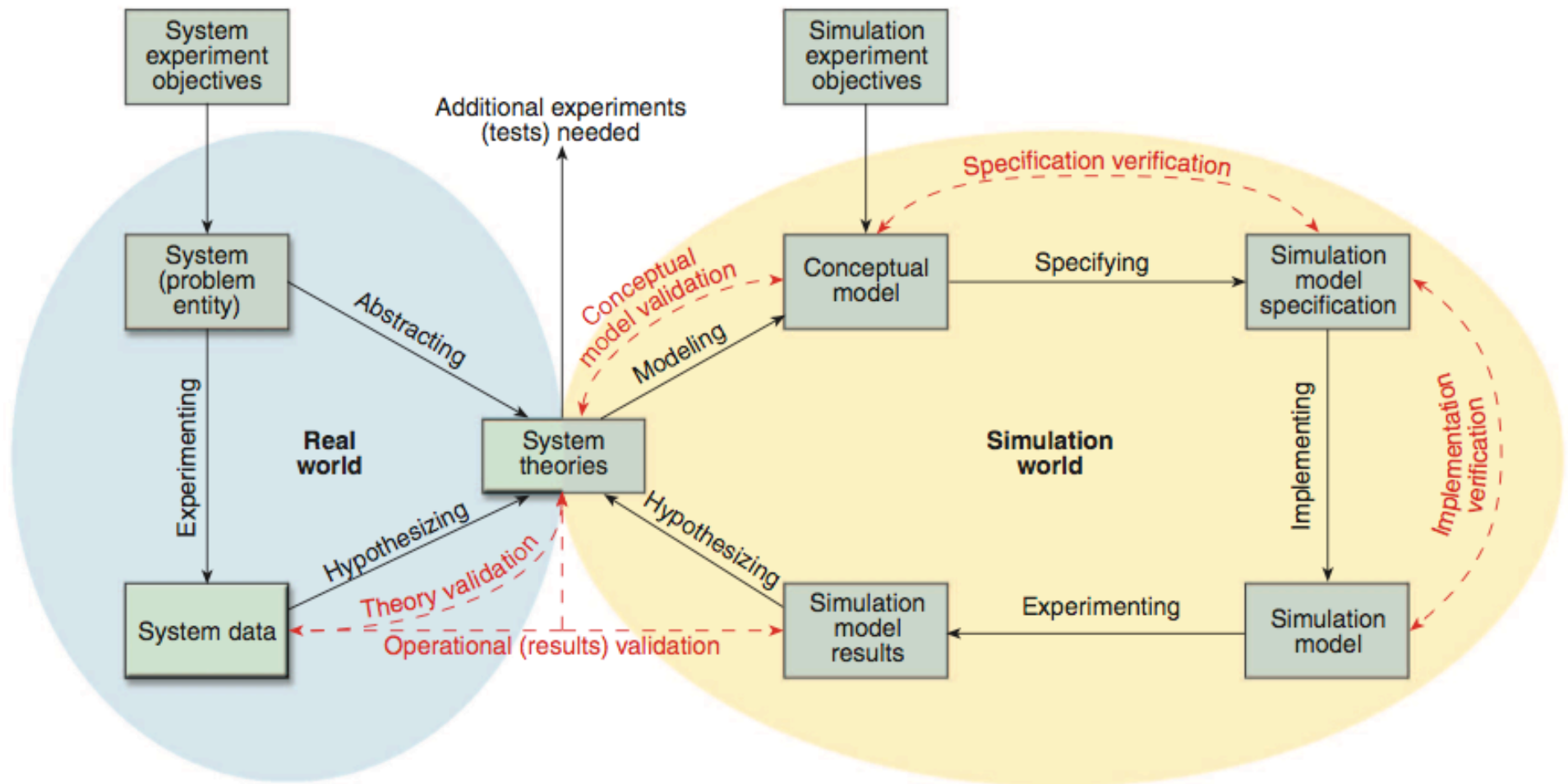
**Jeffrey C. Grossman**  
**Elif Ertekin**

# *Accuracy and Validation*

- Verification and validation (V&V) are processes that help to ensure that models and simulations are correct and reliable.
- Verification: “Did I build the thing right?”
  - Have the model and simulation been built so that they fully satisfy the developer’s intent?
- Validation: “Did I build the right thing?”
  - Will the model or simulation be able to adequately support its intended use? Is its fidelity appropriate for that?

# Accuracy and Validation

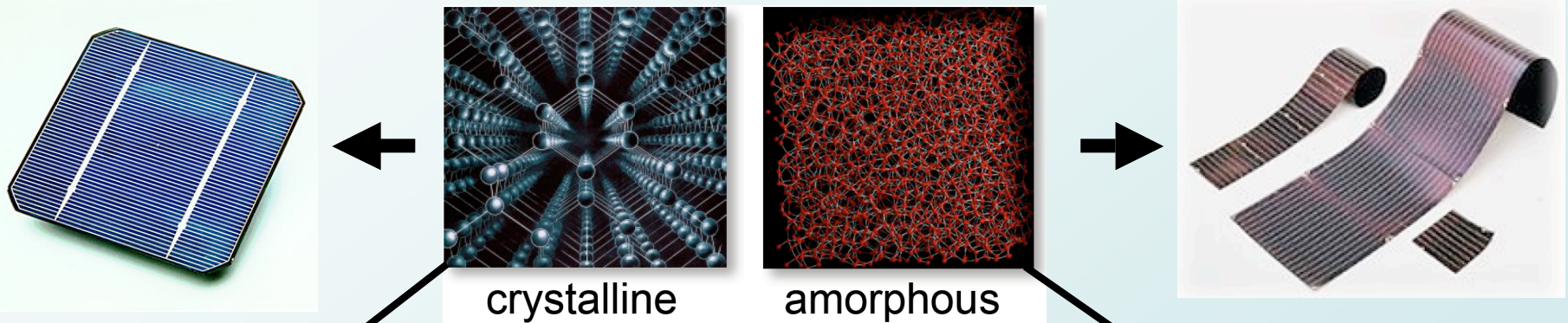
- V&V must be easy, right? Sure, see below:



# *Accuracy and Validation*

- How important is V&V?
- Well, at least one of them is in our case (we often assume the other one is ok).
- Validation, that is.
- That would be, validation is the one we need to worry about. Let's discuss.
- And **both** are becoming part of grant solicitations.

# Amorphous vs. Crystalline Silicon Solar Cells



- Gap: 1.12 eV
- Lower absorption coefficient, device  $\sim 100\ \mu\text{m}$
- Mobilities:
  - electron:  $250\ \mu\text{m}$  in 1 ns
  - hole:  $250\ \mu\text{m}$  in 3 ns

- Gap: 1.6-1.8 eV
- High absorption coefficient, device  $\sim 1\ \mu\text{m}$
- Mobilities:
  - electron:  $0.25\ \mu\text{m}$  in 1 ns
  - hole:  $0.25\ \mu\text{m}$  in 200 ns

# Staebler-Wronski Effect (SWE)

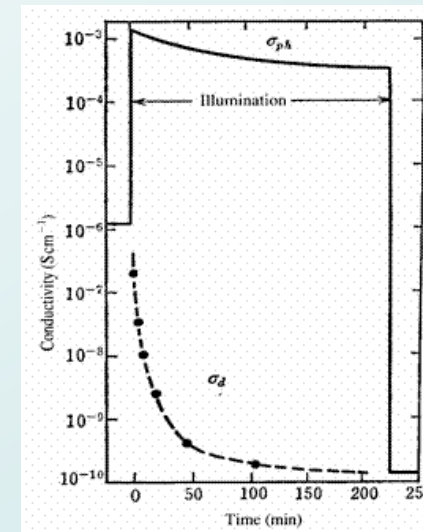
Staebler and Wronski found that under illumination, a-Si:H films suffer from strongly reduced photoconductivity and dark conductivity.

These properties return to their as-deposited values after annealing at temperatures above 160 C.

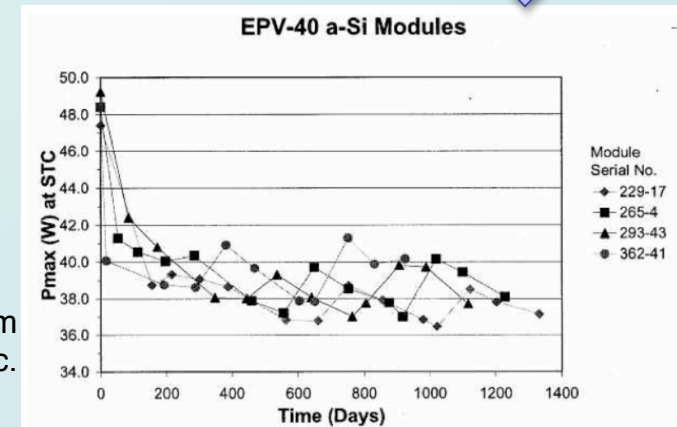
Despite sustained and intense efforts to eliminate SWE it has remained a problem for thirty years.

Severely limits the opto-electronic properties and device performance.

D. Osborn, Spectrum Energy, Inc.

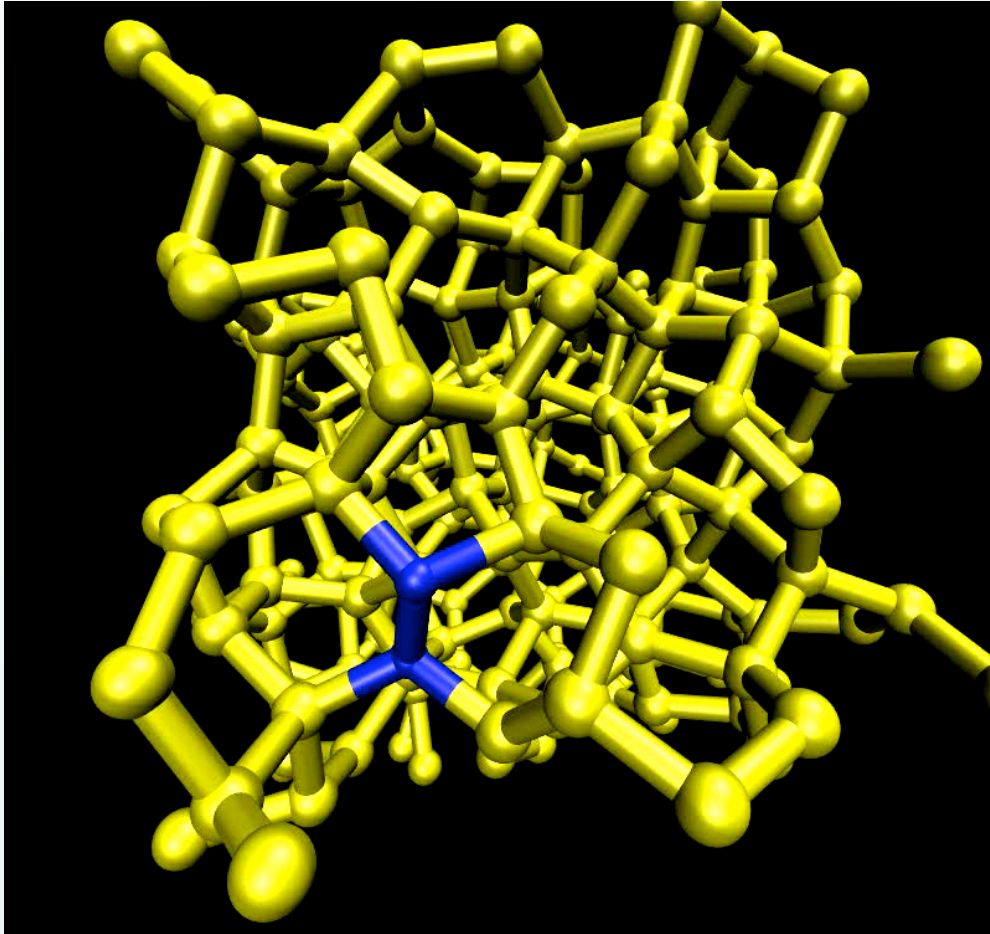


D.L. Staebler and C.R. Wronski, Appl. Phys. Lett. 31, 292-294 (1977).





# Bond Switches



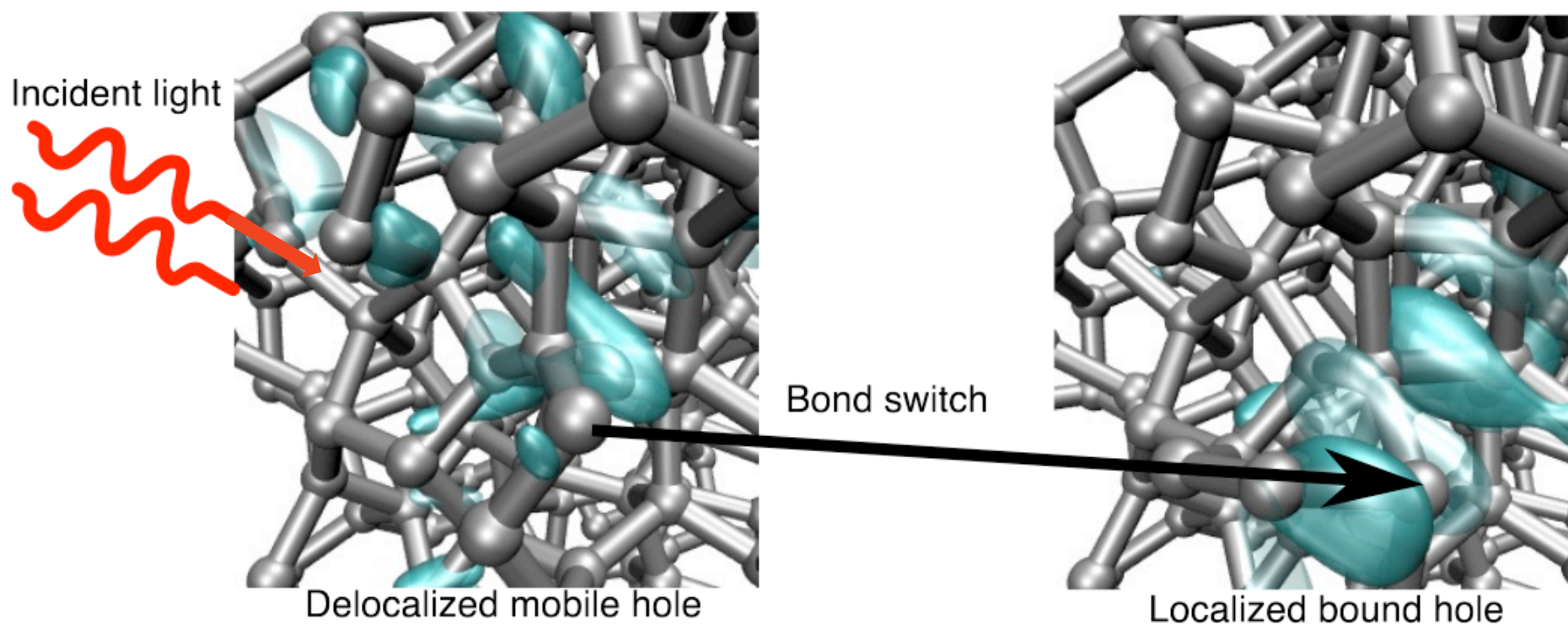
Rotation of a single Si-Si bond

All atoms remain 4-fold coordinated

Energetic cost in crystalline Si  
 $\sim 4.5$  eV

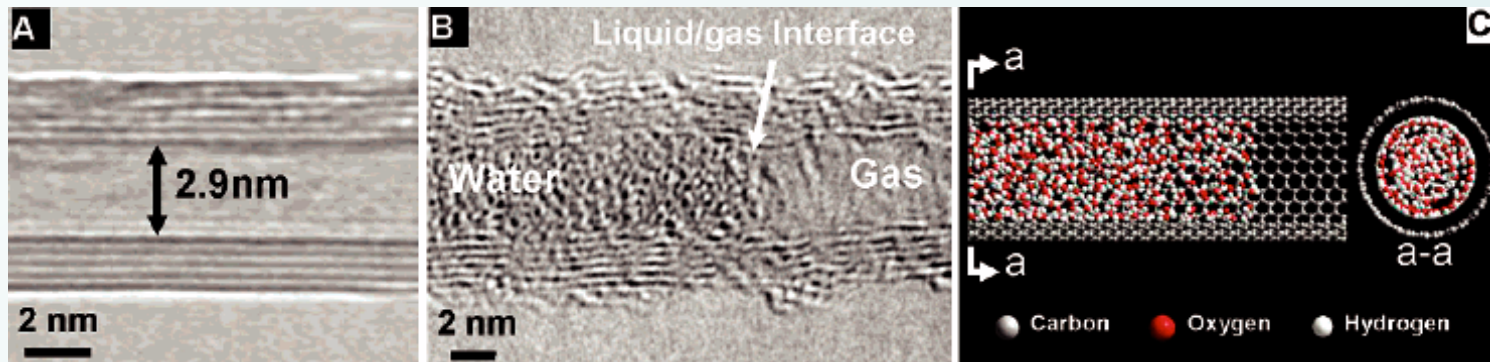
Energetic cost in amorphous Si much lower, as little as 0 eV

# New Microscopic Picture of SWE





# Confined Water



Naguib et al Nanoletters 4, 2237 (2004)

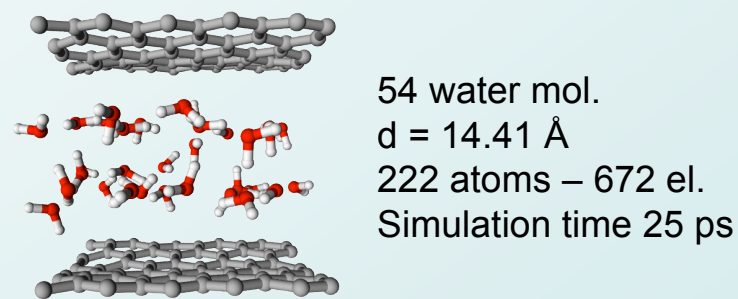
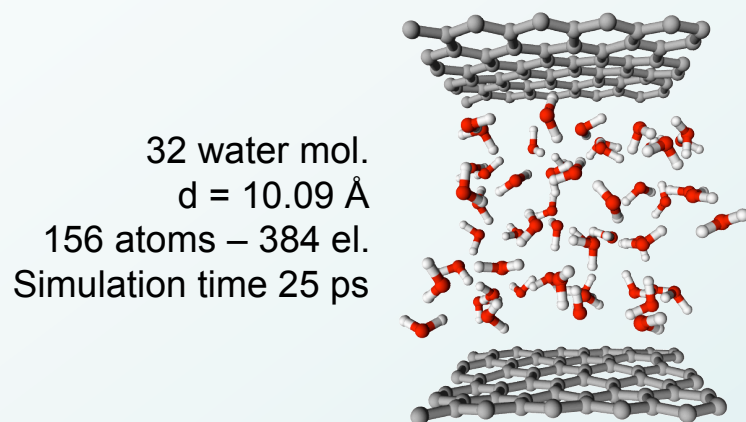
Still many open issues:

New Ice-phase stabilized in confined media at room T?

Will viscosity remain close to bulk value?

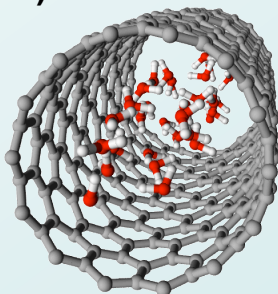
# Confined Water in Hydrophobic Channels

Distinguish between surface and confinement effects



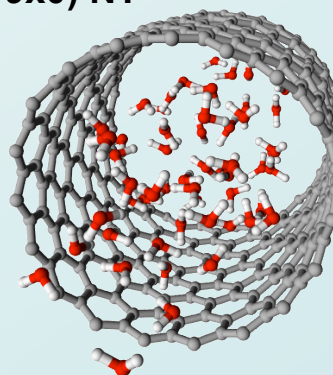
**(14x0) NT**

34 water mol. in (14x0) NT  
438 atoms – 1616 el.  
 $d = 11.1 \text{ \AA}$   
Simulation time 20 ps



**(19x0) NT**

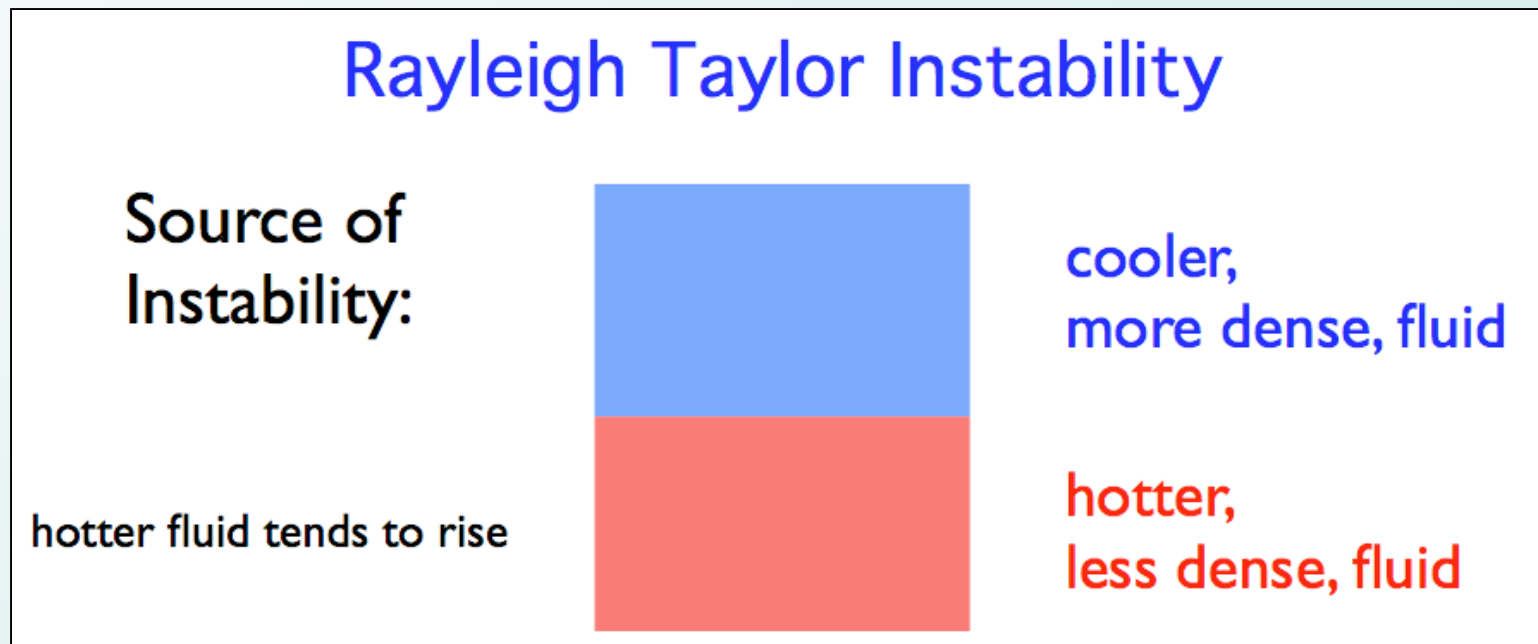
54 water mol. in (19x0) NT  
 $d = 15 \text{ \AA}$   
466 atoms – 1648 el.  
Simulation time 20 ps



# *Rayleigh-Taylor Instability*

This awesome example comes from Leo P. Kadanoff's presentation entitled "The Good, the Bad, and the Awful -- Scientific Simulation and Prediction"

You can listen to and watch (yes, audio and video) his half hour presentation on the nanoHUB. Highly recommended!



## *Rayleigh-Taylor Instability*

- Idea: occurs anytime a dense, heavy fluid is accelerated into a light fluid or lesser density
- Slight perturbations to plane parallel interfaces are unstable ...fingers grow into sets of inter-penetrating fingers
- Observed in weather inversions, salt domes, star nebulae
- How to model this process? Requires solving hydrodynamics equations.

# Rayleigh-Taylor Instability

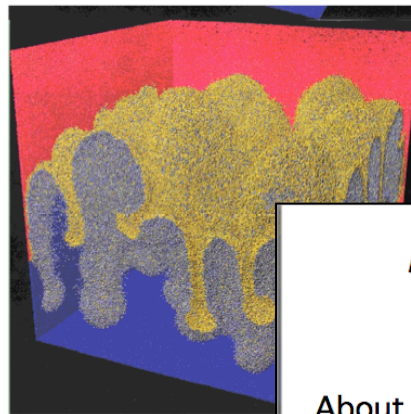
This awesome example comes from Leo P. Kadanoff's presentation entitled "The Good, the Bad, and the Awful -- Scientific Simulation and Prediction"

## The Raleigh Taylor Instability.

Small deviations from perfect surface flatness triggers an instability. The two fluids penetrate into one another. Analysis (dimensional and RG arguments) suggest a penetration distance

$$h = \alpha A g t^2$$

with A being the Atwoods number (density contrast) and  $\alpha$  being dimensionless---and also **Universal (!?)**.

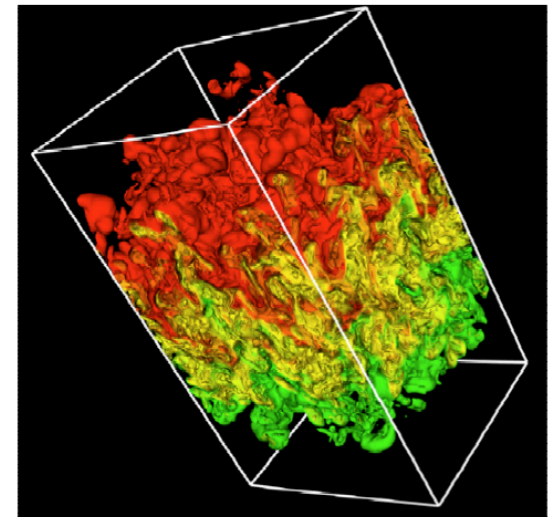


Computer Simulations V2.9--For Berkeley

Kai Kadau...Berni Alder, "Nanohydrodynamics", '04. 1.3\*10<sup>8</sup> particles

$$h = \alpha A g t^2$$

About 15 groups have measured or calculated  $\alpha$ . Their results are important for us (a DOE supported astrophysics group) because the instability occurs on the surface of an exploding star.



Fluid Mechanics Simulation of RT instability. "On Validating an Astrophysical Simulation Code". A. C. Calder, et al. *Astrophys.J.Supp.* **143** 201-230 (2002). The value of  $\alpha$  differs from previous picture by a factor of two.

Computer Simulations V2.9--For Berkeley

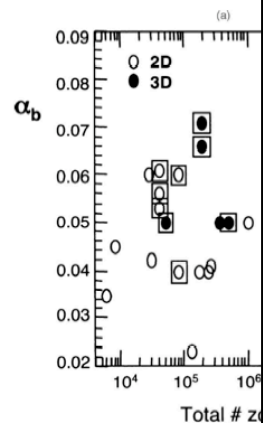
10-5-07



# Rayleigh-Taylor Instability

This awesome example comes from Leo P. Kadanoff's presentation entitled "The Good, the Bad, and the Awful -- Scientific Simulation and Prediction"

## Summary of Different Studies

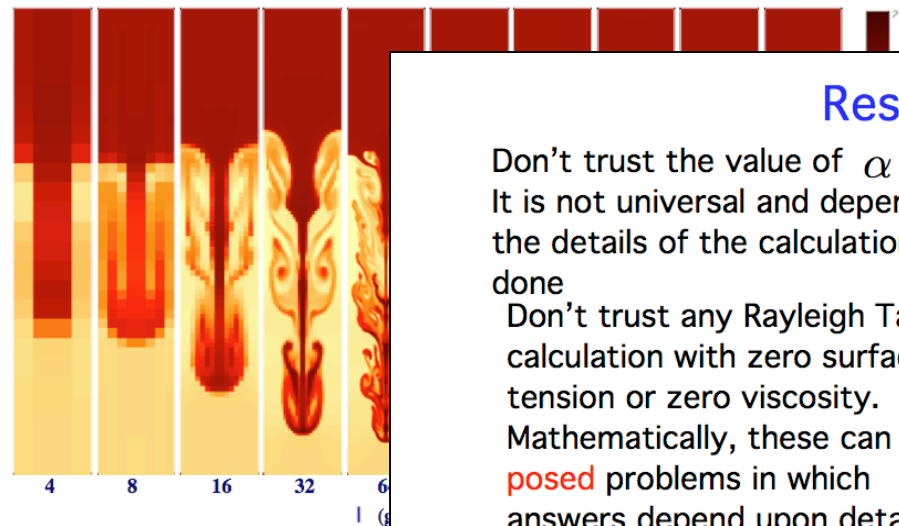


A comparative study of the turbulent three-dimensional numerical simulation of the Rayleigh-Taylor instability  
Guy Dimonte, et al. Physics of Fluids

The 'b' refers to the bubble, which fluid penetrates as spikes.

Computer Simulations V2.9--For Berkeley

## Resolution Study $d=2$ denser fluid on top color codes for density



Computer Simulations V2.9--For Berkeley

10-5-0

## Result

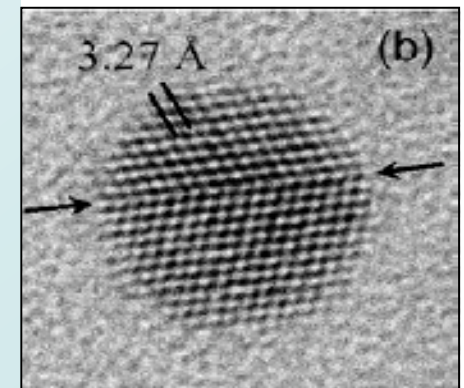
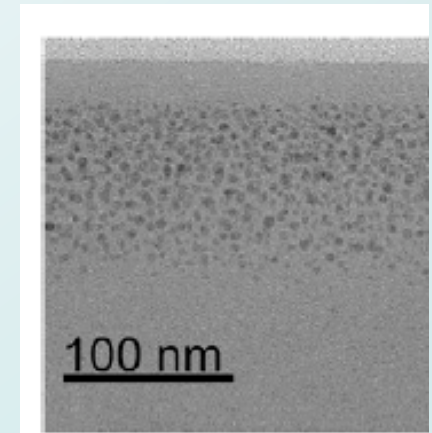
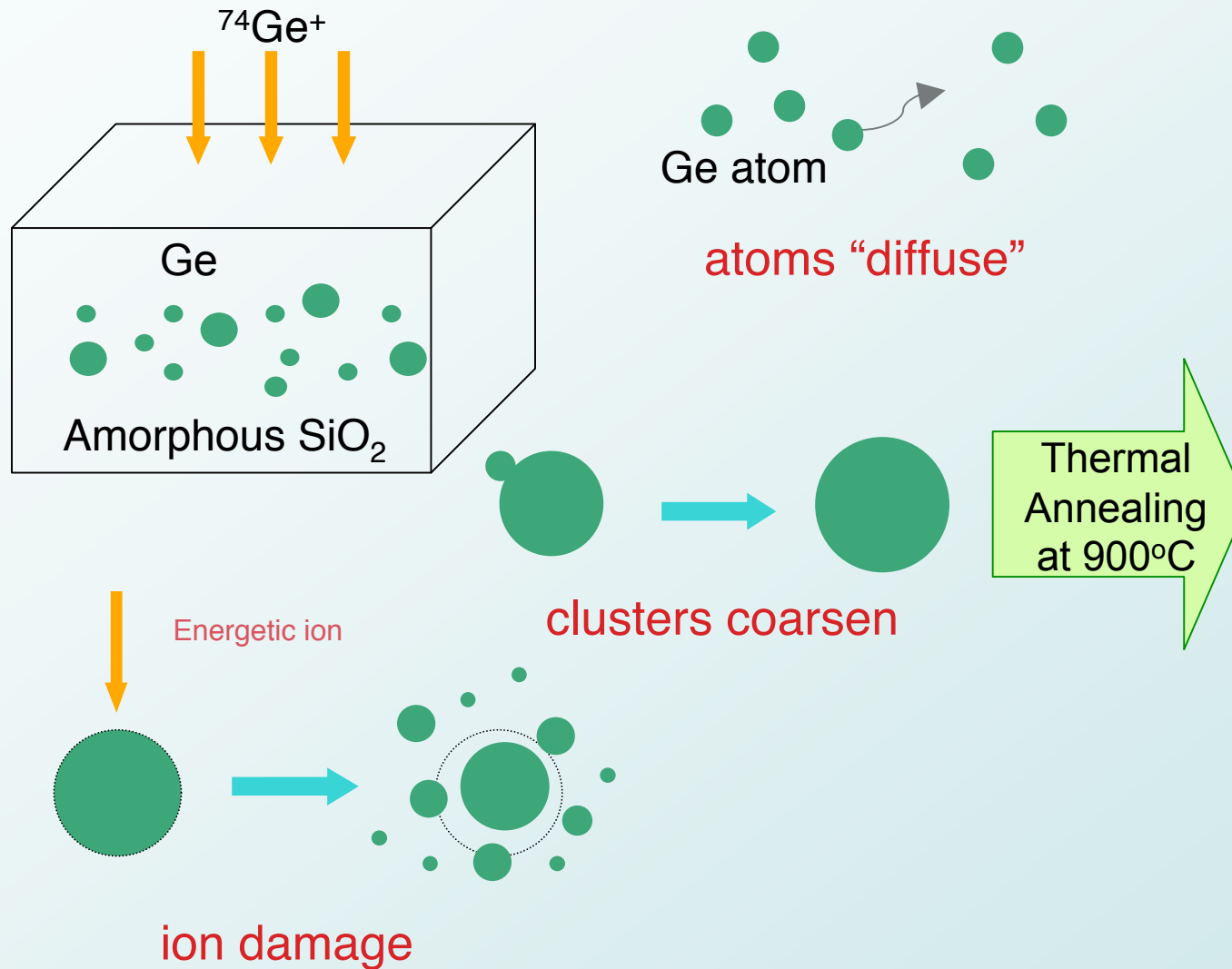
Don't trust the value of  $\alpha$   
It is not universal and depends on the details of the calculation being done  
Don't trust any Rayleigh Taylor calculation with zero surface tension or zero viscosity.  
Mathematically, these can give ill posed problems in which answers depend upon details of what happens at the earliest time.

Computer Simulations V2.9--For Berkeley

10-5-07

# *Ion Beam Synthesis of Nanocrystals*

Courtesy: C. W. Yuan, D. C. Chrzan



I.D. Sharp, *et al.* J. Appl. Phys., 97, 124316 (2005)

## *Goals & Outline*

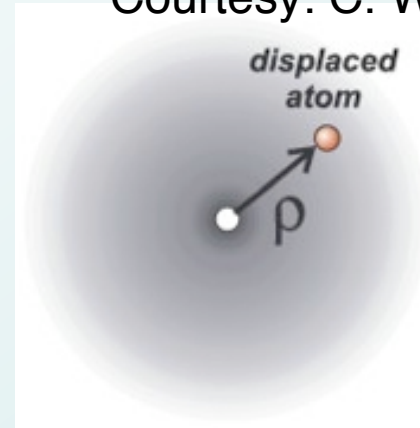
Courtesy: C. W. Yuan, D. C. Chrzan

- Goal: Quantitative model for ion beam synthesis of nanocrystals
  - predict: cluster size distributions
  - identify: experimental parameters that control distribution
- How would you do it??

# Kinetic Processes - Fragmentation

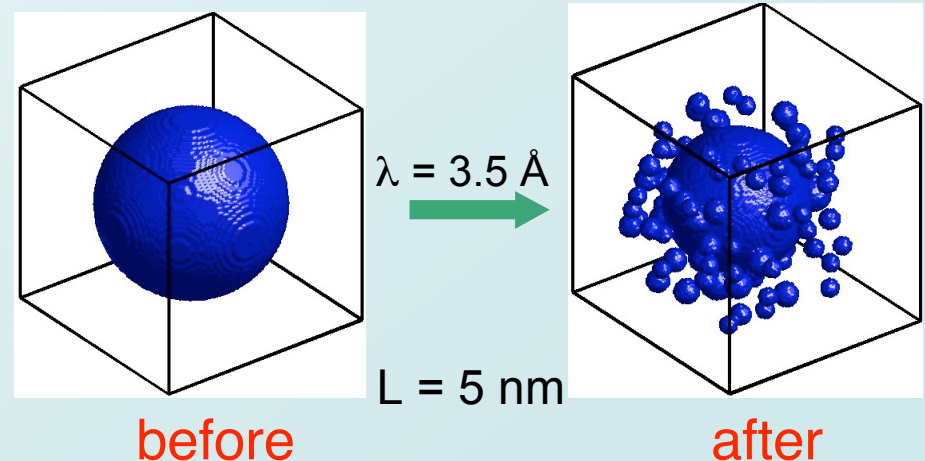
- statistical approach
  - ion collision displaces atoms randomly/simultaneously
    - displacement probability  $f(\rho)$
    - $\lambda$  determined through TRIM.
  - rapid “reclustering”
- power law fragment size distribution
  - MD simulation of ion-induced fragmentation of Au cluster reported by Kissel & Urbassek.
  - incorporate into rate equations

Courtesy: C. W. Yuan, D. C. Chrzan



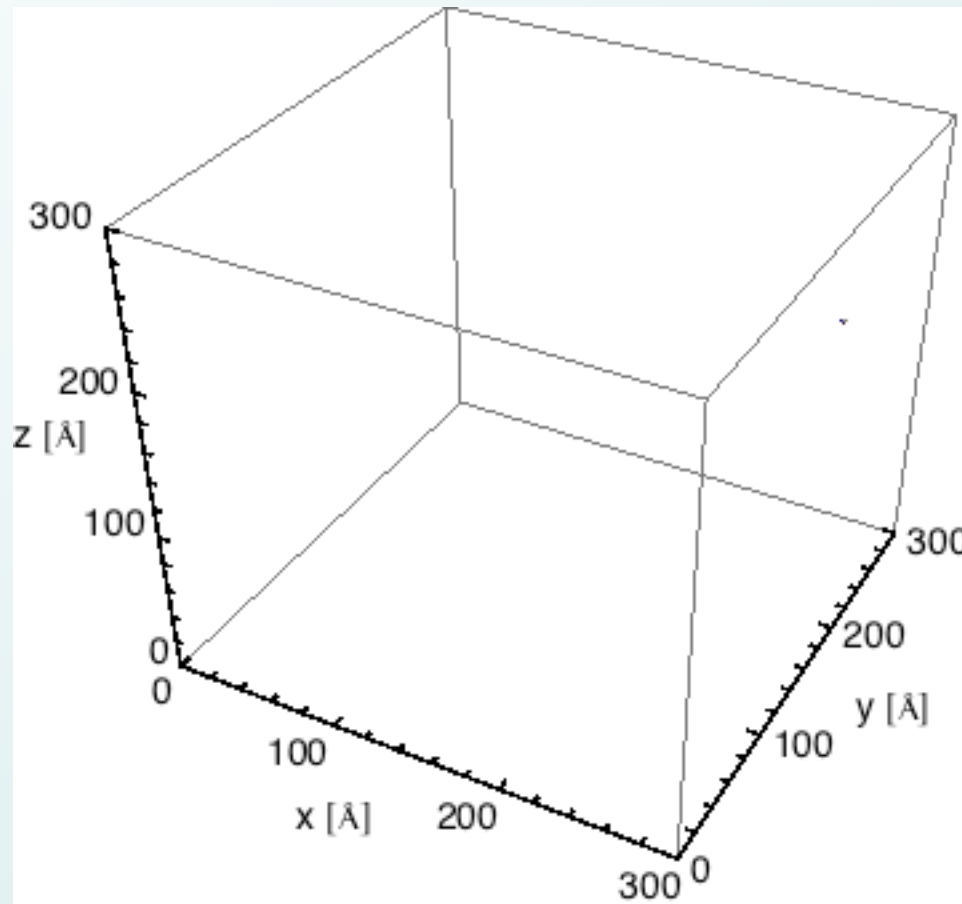
$$f(\rho) \propto \exp\left(\frac{-\rho}{\lambda}\right)$$

K. H. Heinig, *et al.* Appl. Phys. A 77, 17-25 (2003)



# *Results - kinetic Monte Carlo*

Courtesy: C. W. Yuan, D. C. Chrzan

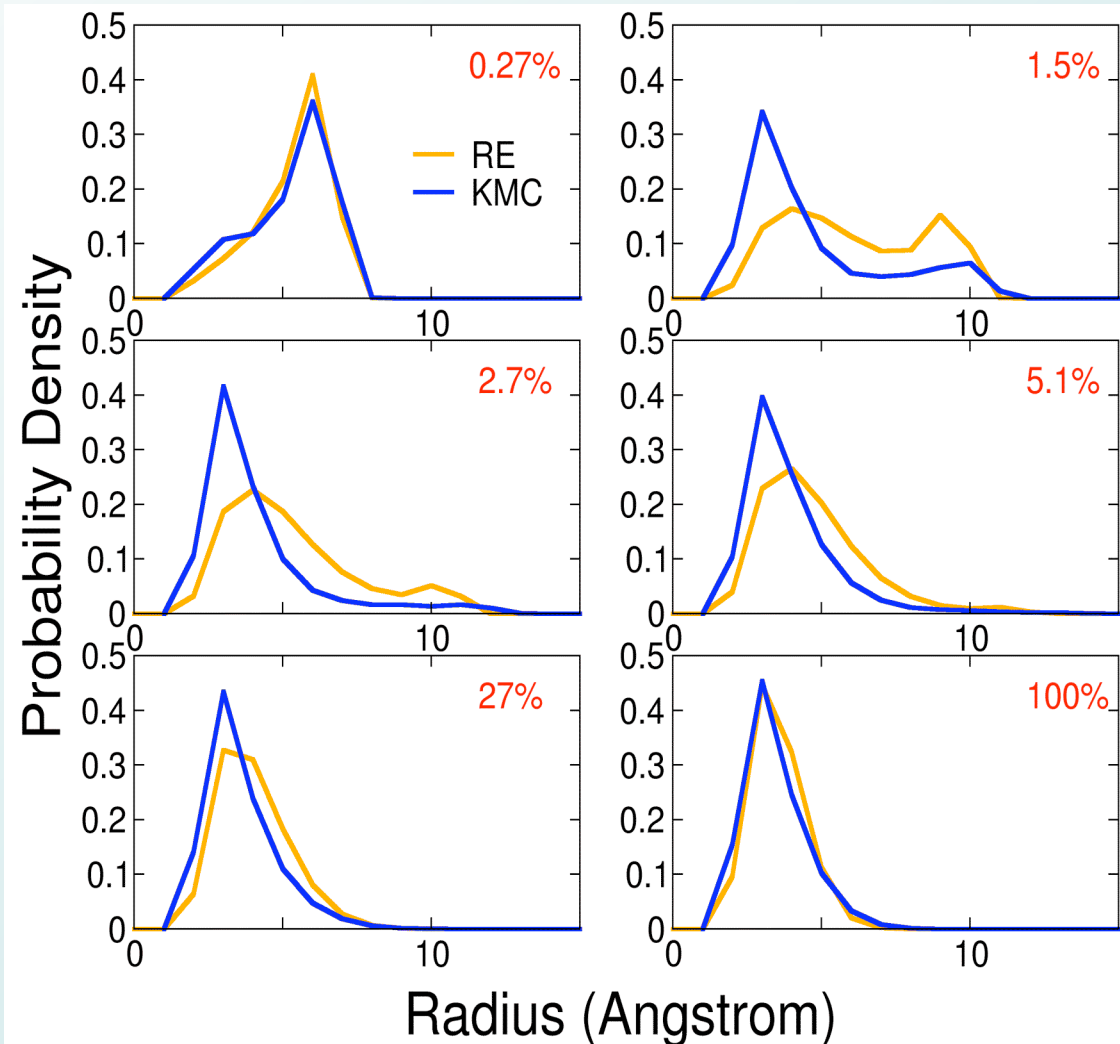




# KMC vs RE

Courtesy: C. W. Yuan, D. C. Chrzan

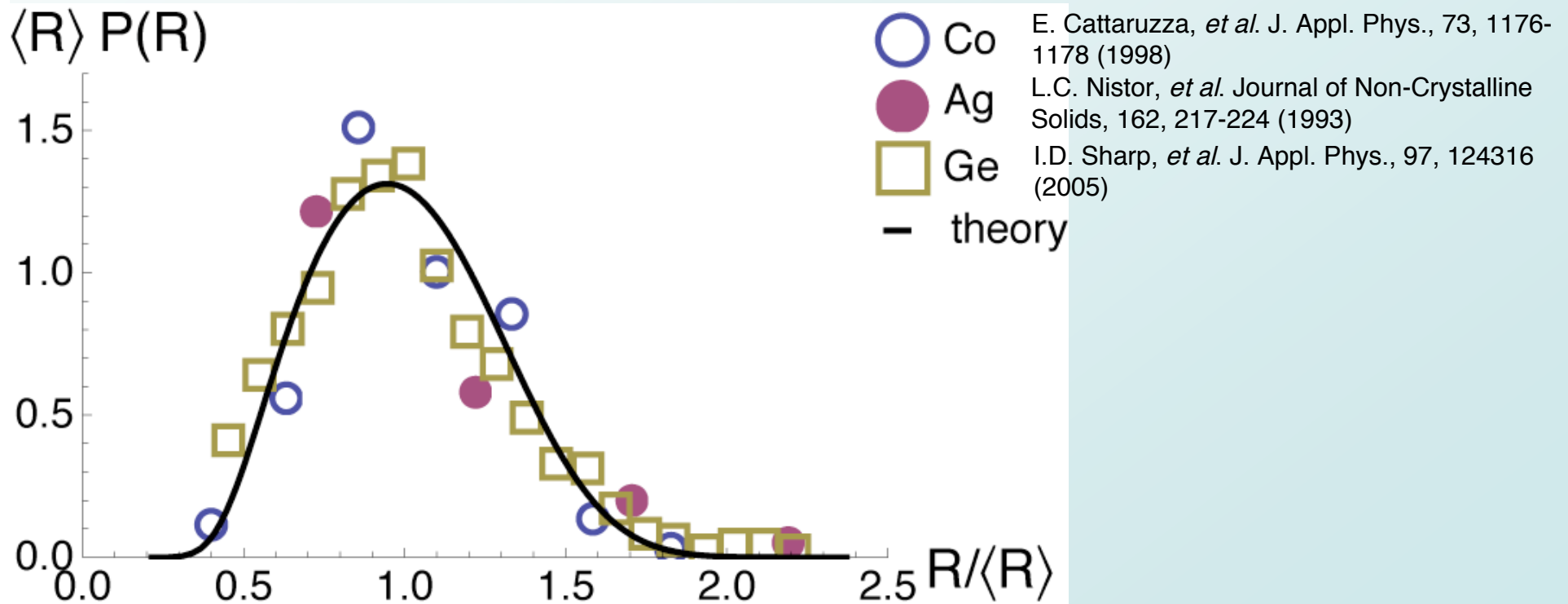
- $F = 1.5 \times 10^{12} \text{ cm}^{-2} \text{ s}^{-1}$
- $D = D_0 = 6.5 \times 10^{10} \text{ cm}^2 \text{ s}^{-1}$
- $\gamma = 0.2 \text{ J m}^{-2}$
- $N = 4 \times 10^{16} \text{ cm}^{-2}$
- KMC and RE display good agreement
  - log-normal-like size distribution!
- Simulations approach a steady-state
- Use RE to explore key parameters that govern size distribution
  - Implantation rate vs. relaxation rate
  - Interface energy



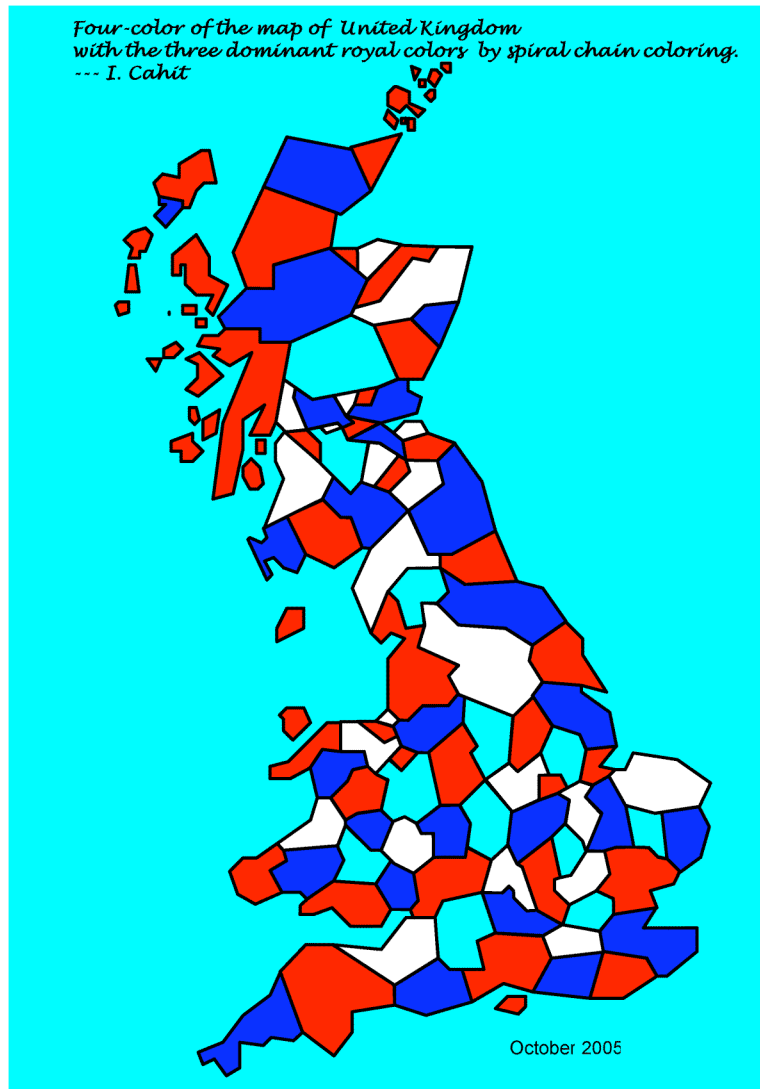
## Theory vs. Experiment

Courtesy: C. W. Yuan, D. C. Chrzan

- $D \sim 10^2 D_0$  agrees well with several experimentally-observed as-implanted size distribution
- Indicates that the value of  $F/D$  may be intrinsic to the implantation process



# Four Colored Map



<http://www.emu.edu.tr/%7Ecahit/>

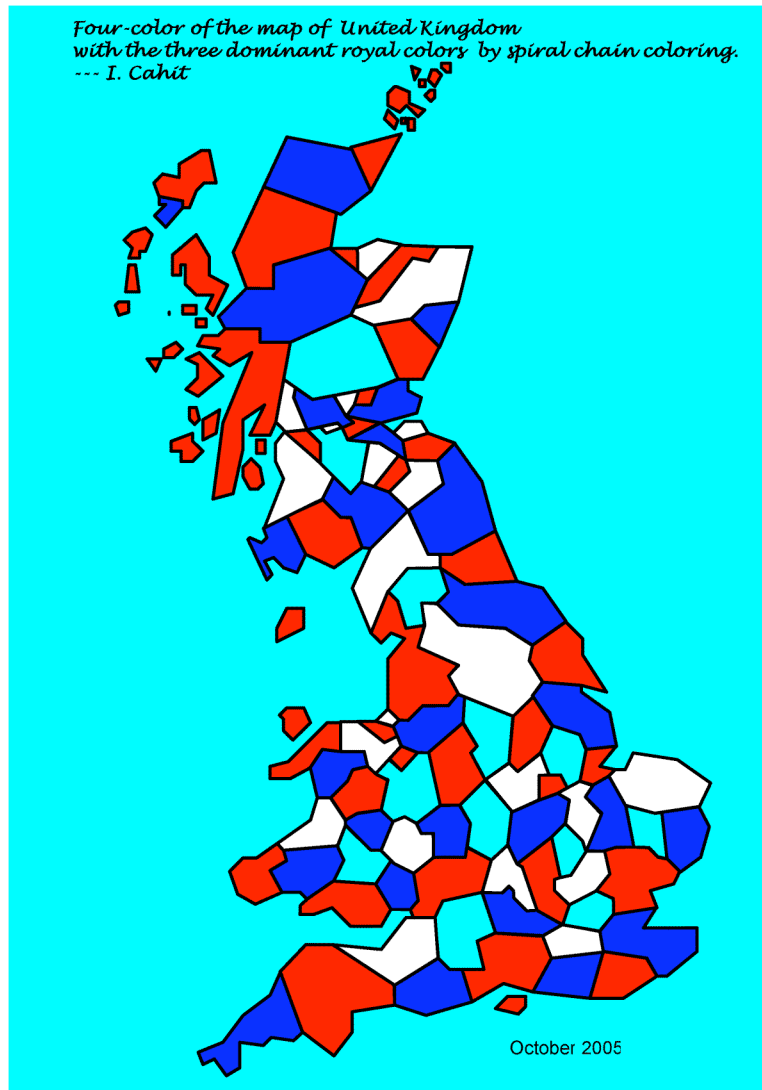
Theorem: given any plane separated into connected regions, the regions may be colored using no more than four colors in such a way that no two adjacent regions receive the same color

First proposed in 1852 when a student realized while coloring the counties of England that only four colors were needed

Not proven until 1976 by mathematicians at U. of Illinois.

How might one go about proving this?

# Four Colored Map



<http://www.emu.edu.tr/%7Ecahit/>

Several failed attempts at analytically proving the theorem ...

In fact, this is considered to be the first major theorem proven with a computer

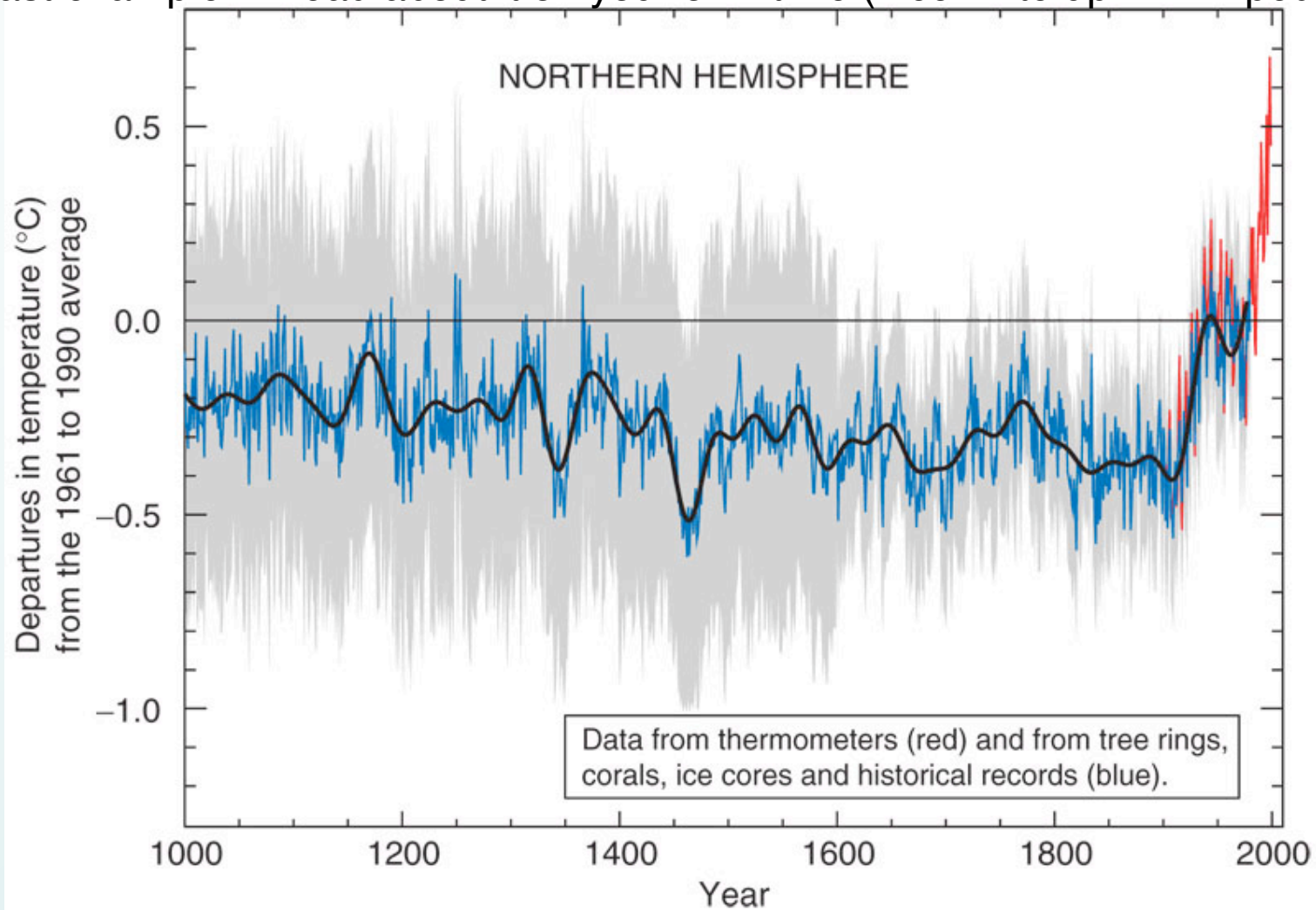
Thus, it is not accepted by all mathematicians because it is unfeasible for a human to verify by hand - must trust the compiler and the hardware

Basic approach: the set of all possible maps can be reduced to 1476 “reducible configurations”. A computer was used to verify these configurations.

By the way, there is no extension of the theorem to three-dimensional space.

# Hockey Stick Controversy

One last example ... read about it on your own time (nice write up in Wikipedia)



“Hockey stick” graph shown in 2001 IPCC report, showing data from Mann, Bradley, & Hughes, *Nature*, 1998.

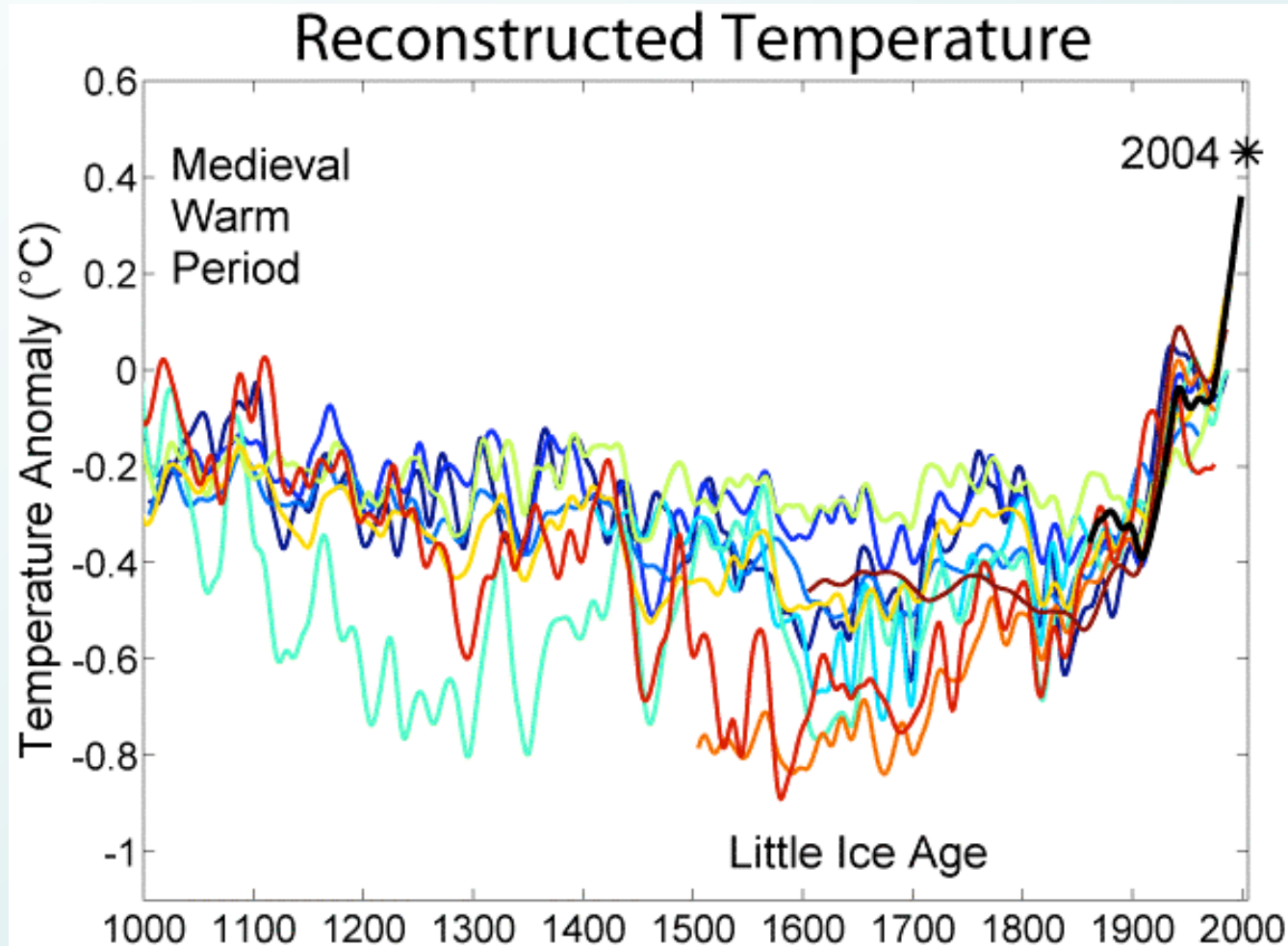


## *Hockey Stick Controversy*

- Issues raised relate to:
  - Validity of various temperature proxies
  - Reasonableness of the Global Climate Model used
  - Implementation of “principal component method” used to reduce dimensionality of large data sets for simpler analysis
- Ensuing debate involving National Research Council, National Academy of Sciences, American Geophysical Union, Congress

# Hockey Stick Controversy

One last example ... read about it on your own time (nice write up in Wikipedia)



Reconstructions of Northern Hemisphere temperatures according to older (blue), newer (red), and recorded data (black)

# ***Hockey Stick Controversy***

## **Paleoclimate findings by the IPCC before and after the Hockey Stick Controversy:**

Before: 2001 (page 2)[53]

" proxy data for the Northern Hemisphere indicate that the increase in temperature in the 20th century is likely to have been the largest of any century during the past 1,000 years. It is also likely that, in the Northern Hemisphere, the 1990s was the warmest decade and 1998 the warmest year."

After: Current SPM statement from 2007 (page 10)[54]

"“Average Northern Hemisphere temperatures during the second half of the 20th century were very likely higher than during any other 50-year period in the last 500 years and likely the highest in at least the past 1300 years. Some recent studies indicate greater variability in Northern Hemisphere temperatures than suggested in the TAR, particularly finding that cooler periods existed in the 12 to 14th, 17th, and 19th centuries. Warmer periods prior to the 20th century are within the uncertainty range given in the TAR.”