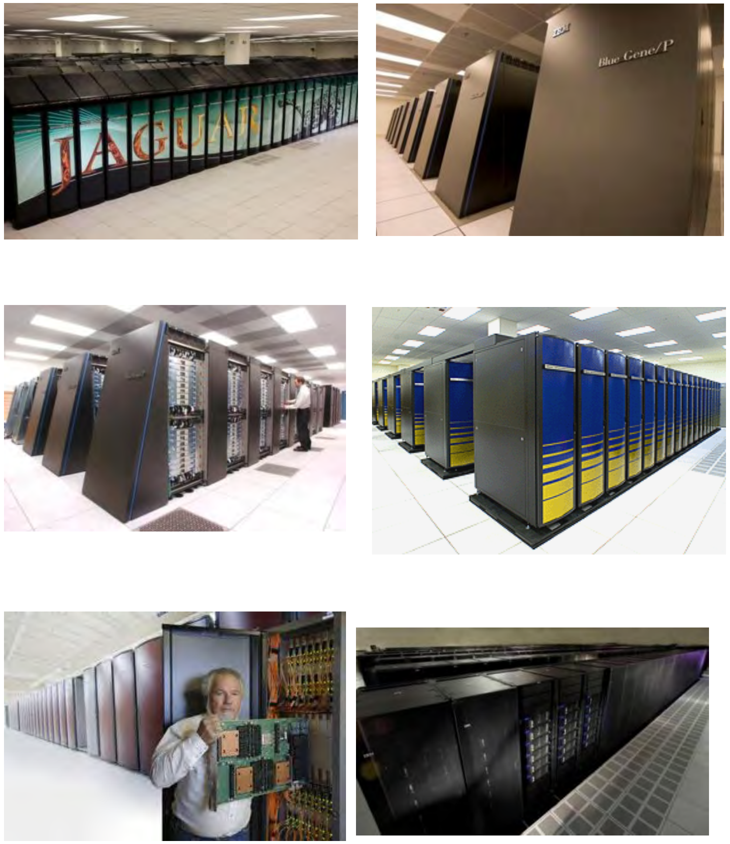
Changing the Game

Simulations Summit
Washington, D.C.
13 October, 2010

DOE provides extreme scale computing: 15 years of world leadership



Top 500 list, June 2010

Machine	Place	Speed (max)	On list Since
Jaguar	ORNL	1.75 PF	2009 (1)
Roadrunner	LANL	1.04 PF	2009 (3)
Dawn	LLNL	0.478 PF	2007 (8)
BG/P	ANL	0.458 PF	2007 (9)
Red Sky (NREL)	SNL	0.434 PF	2010 (10)
Red Storm	LLNL	0.416 PF	2009 (12)
NERSC	LBL	0.266 PF	2008 (18)

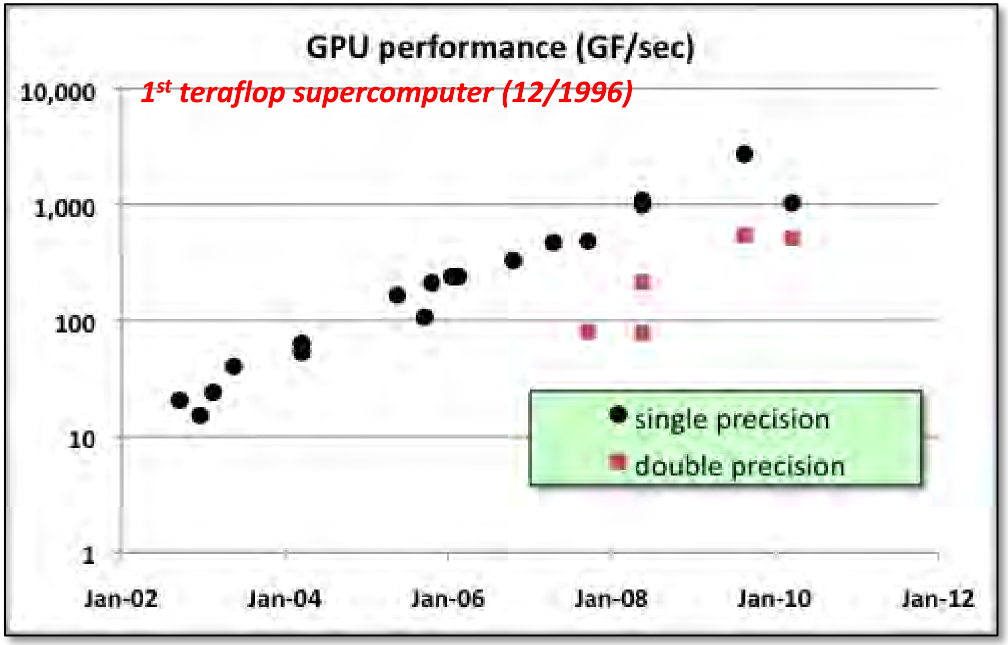
NNSA
Advanced Simulation and Computing

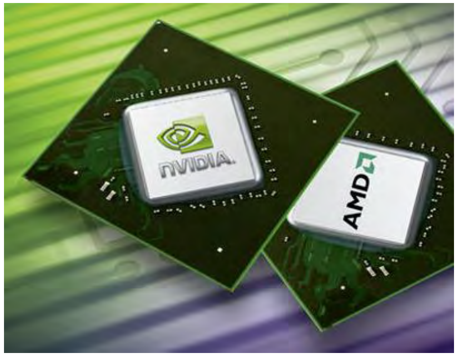
The Office Of
Advanced Scientific Computing Research

Within 5 to 10 years, access to tera and petascale performance will increase dramatically

Today's computers are hybrids between CPUs and GPUs

Accelerators are approaching a teraflop/sec in double precision – effectively putting the performance of the fastest supercompters a decade ago into everyone's hands





The key will be programming a new generation of applications that can run on a thousand cores on the desktop and a billion cores at an exaflop

How is High Performance Computing changing Science and Technology?

1. Climate modeling and prediction
2. Industrial and building design
3. Material and nano-machine properties

How is High Performance Computing changing Science and Technology?

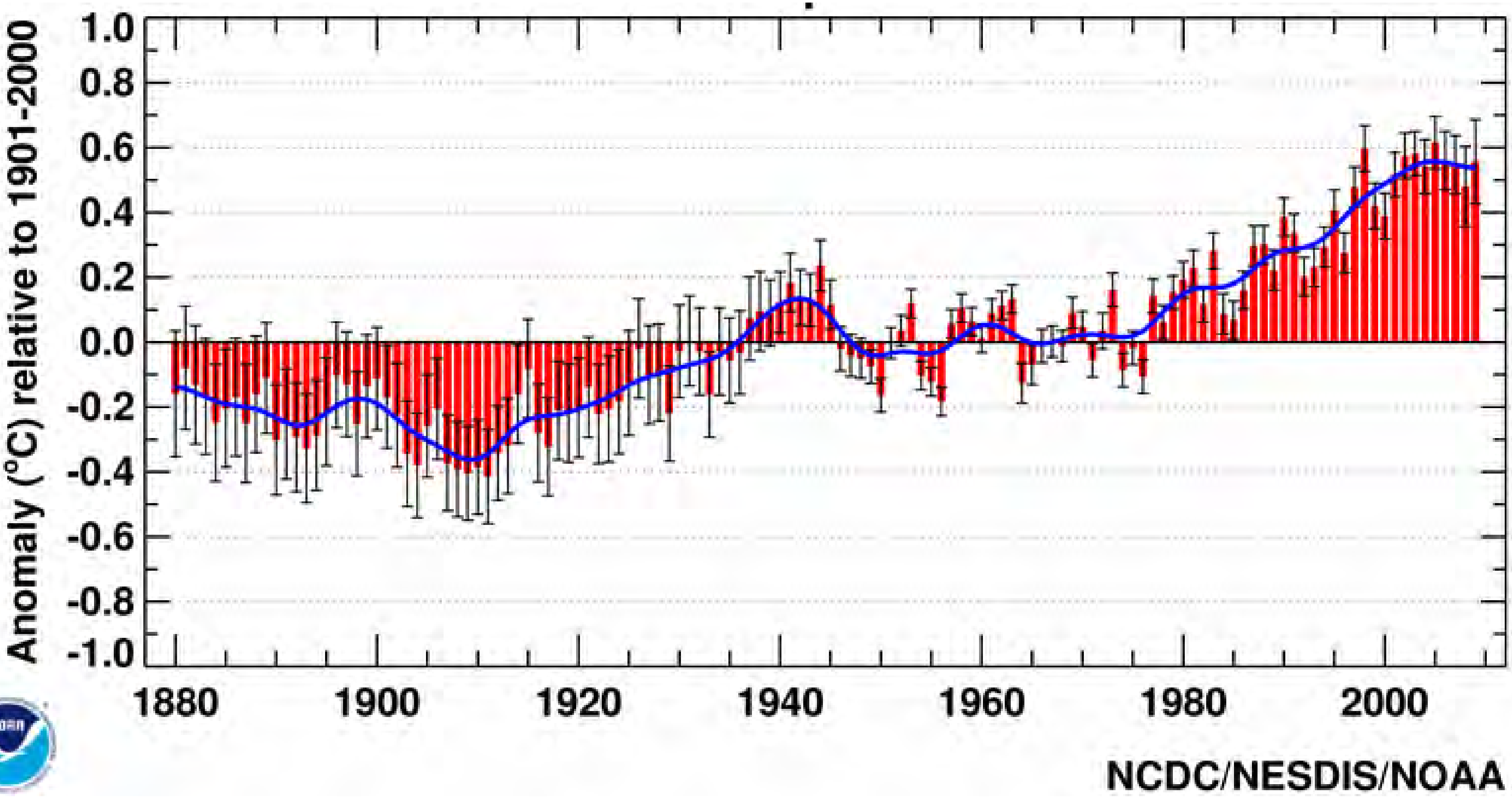
1. Climate modeling and prediction

Scientific Grand Challenges

CHALLENGES IN CLIMATE CHANGE SCIENCE AND THE ROLE OF COMPUTING AT THE EXTREME SCALE

November 6-7, 2008 • Washington D.C.

Temperature Record (1880 – 2009)

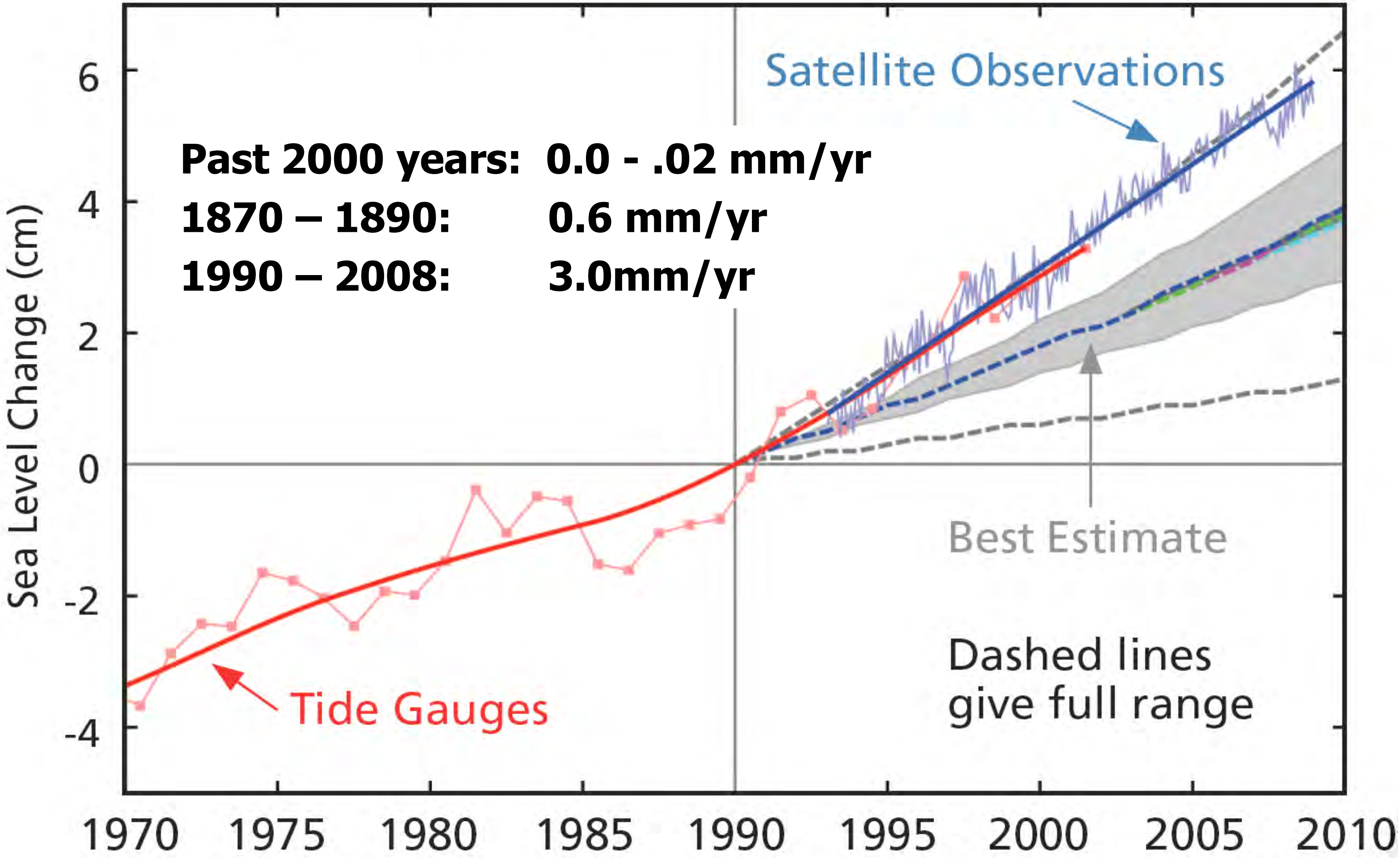


Computational Challenges of Climate Modeling

1. How will the sea level, sea-ice coverage, and ocean circulation change as the climate changes?

Sea level rise

Past 2000 years: 0.0 - .02 mm/yr
1870 – 1890: 0.6 mm/yr
1990 – 2008: 3.0mm/yr

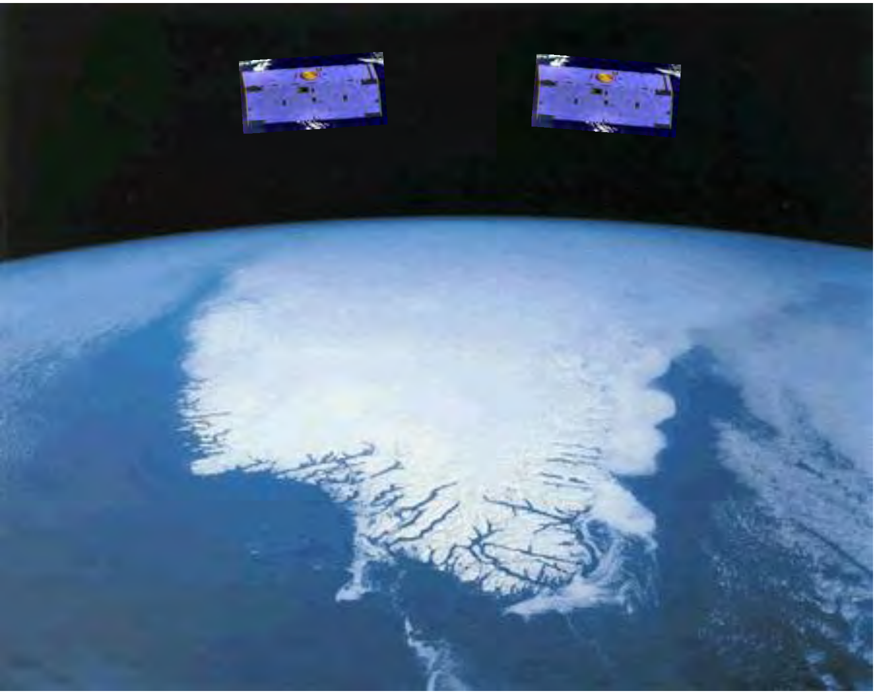


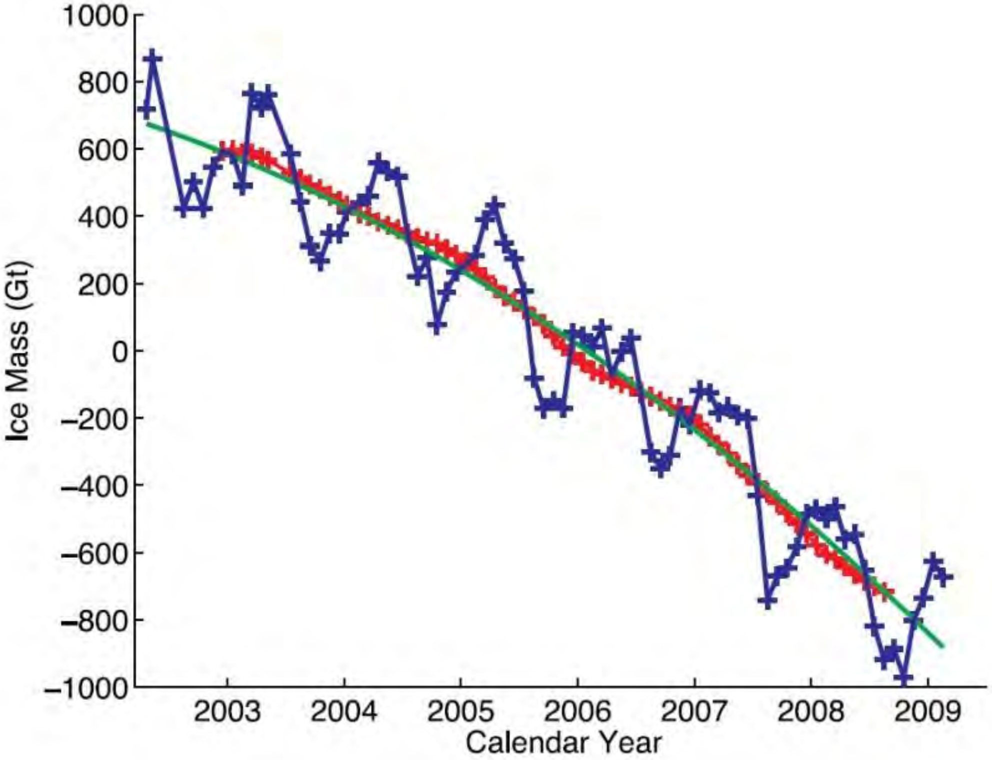
Source: Rahmstorf et al. 2007 and updated by personal communication

The sea level is rising. Past 2000 years: 0.0 - .02 mm/year
Currently 3.0mm/year

Greenland Ice Mass Loss – 2002 to 2009

Ice mass loss from the Greenland and Antarctic ice sheets measured by **GRACE** (Gravity Recovery and Climate Experiment) mission.





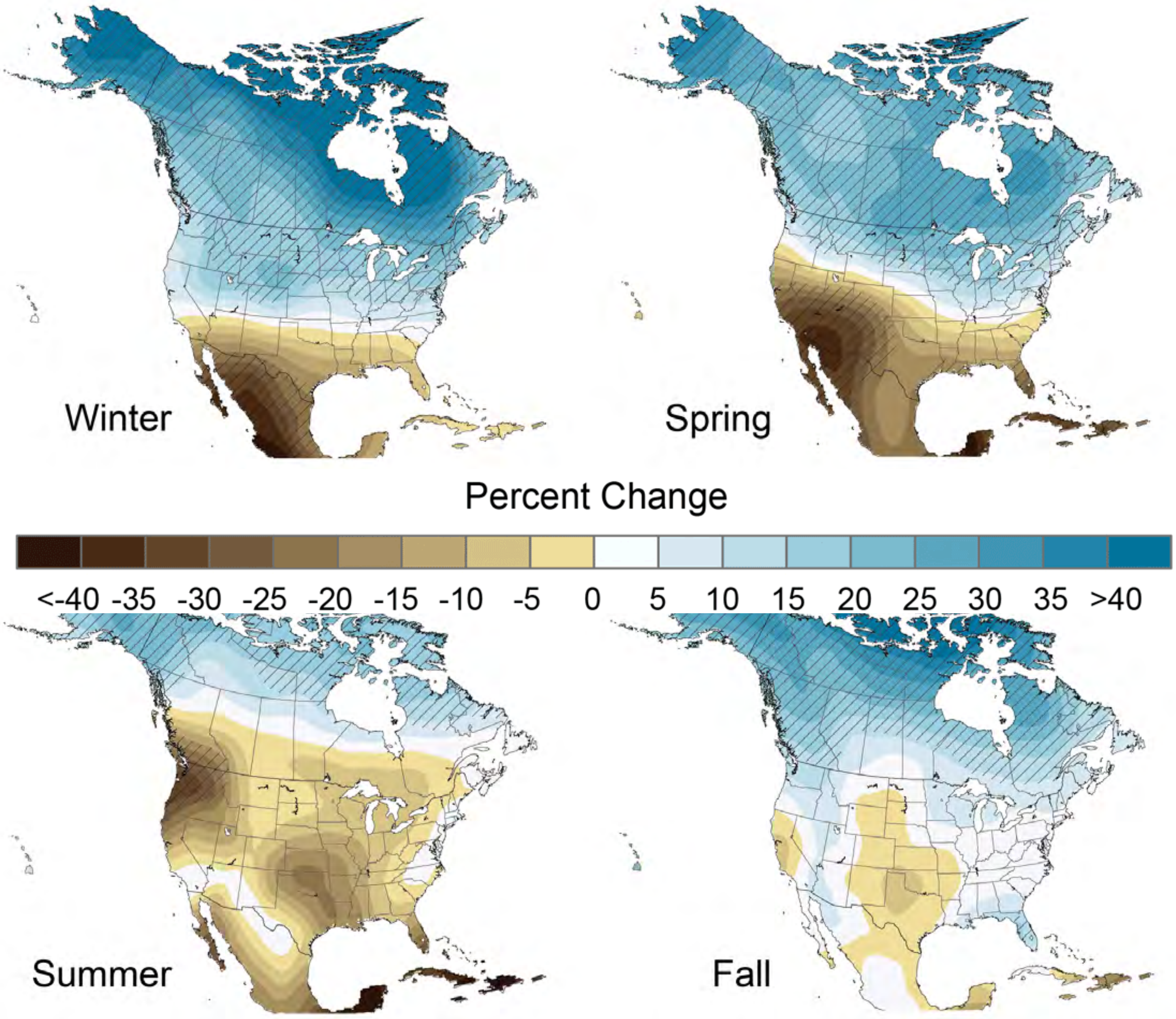
I. Velicogna, GEOPHYSICAL RESEARCH LETTERS, VOL. 36, L19503, doi:10.1029/2009GL040222, 2009

Computational Challenges of Climate Modeling

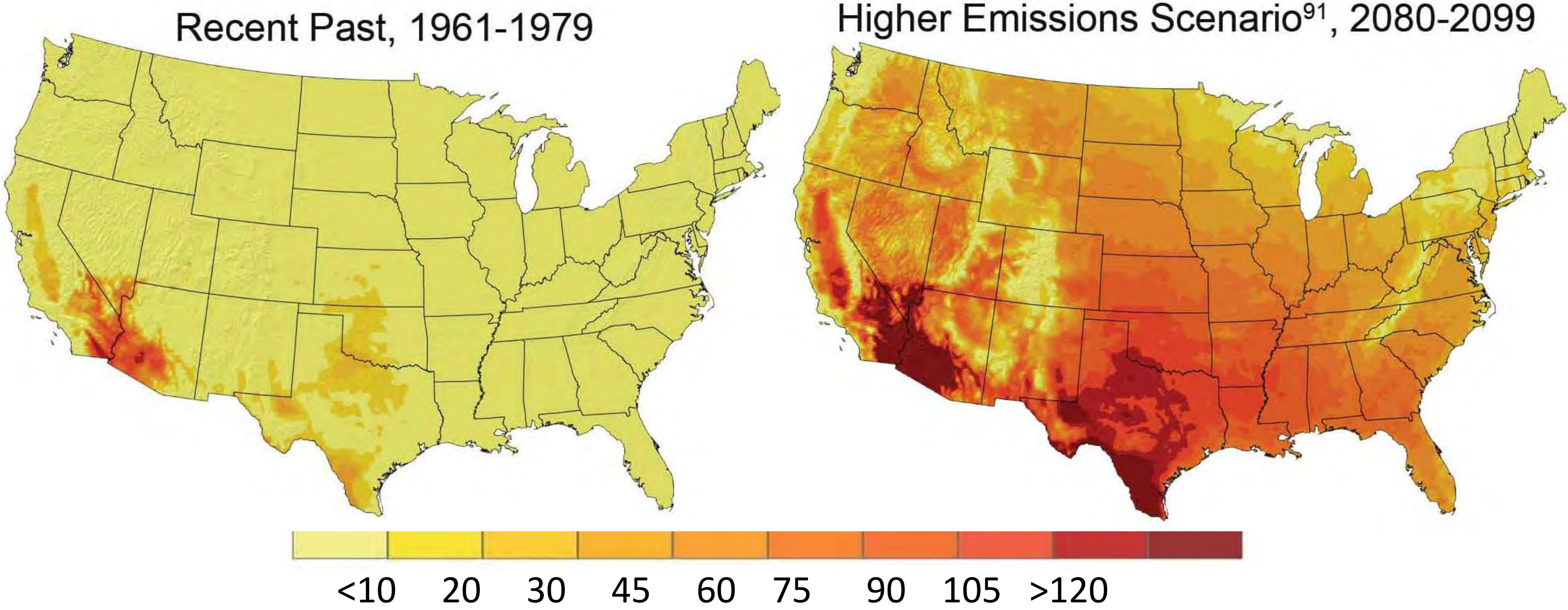
1. How will the sea level, sea-ice coverage, and ocean circulation change as the climate changes?

2. How will the distribution and cycling of water, ice, and clouds change with global warming?

Change in Precipitation by 2080-90s (Higher emissions scenario.) Bread Basket states projected to have 10 -25% less summer rain



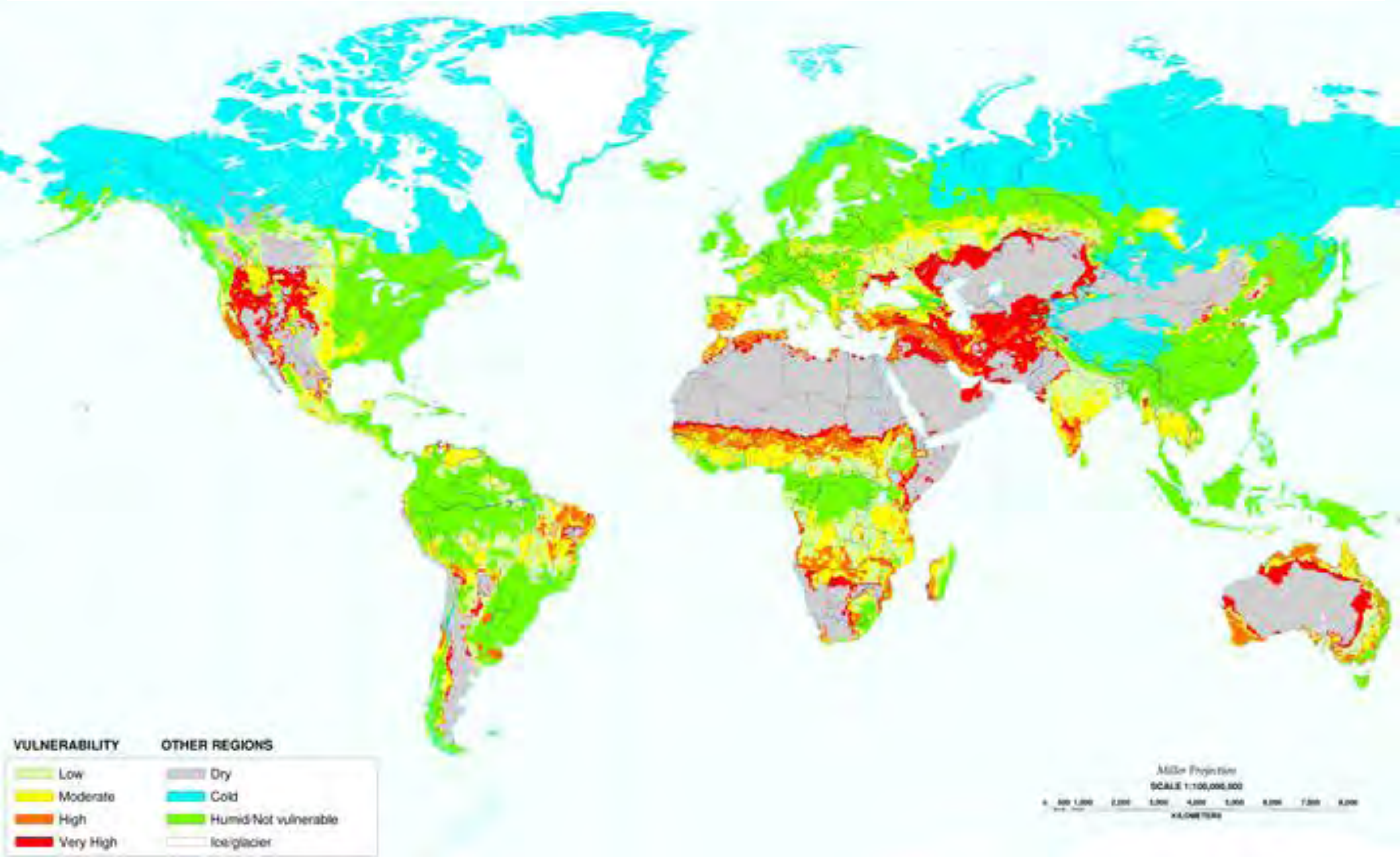
Days above 100º F



Much of the U.S. would go from 0 - 10 days above 100º F to 45 to 70 days per year above 100º F

Source: NOAA U.S. Global Change Research Program

The chance of Fertile Land becoming Desert



The Mid-West Dust Bowl
(1930 -1936)

Computational Challenges of Climate Modeling

1. How will the sea level, sea-ice coverage, and ocean circulation change as the climate changes?

2. How will the distribution and cycling of water, ice, and clouds change with global warming?

3. How will extreme weather and climate change on the local and regional scales?

GFDL Prototype Cloud-Resolving Model


July 17, 2005

Observed Track Information

Hurricane Name: Emily
Category: 5
Highest Winds: 160 mph
Lowest Pressure: 929 mbar

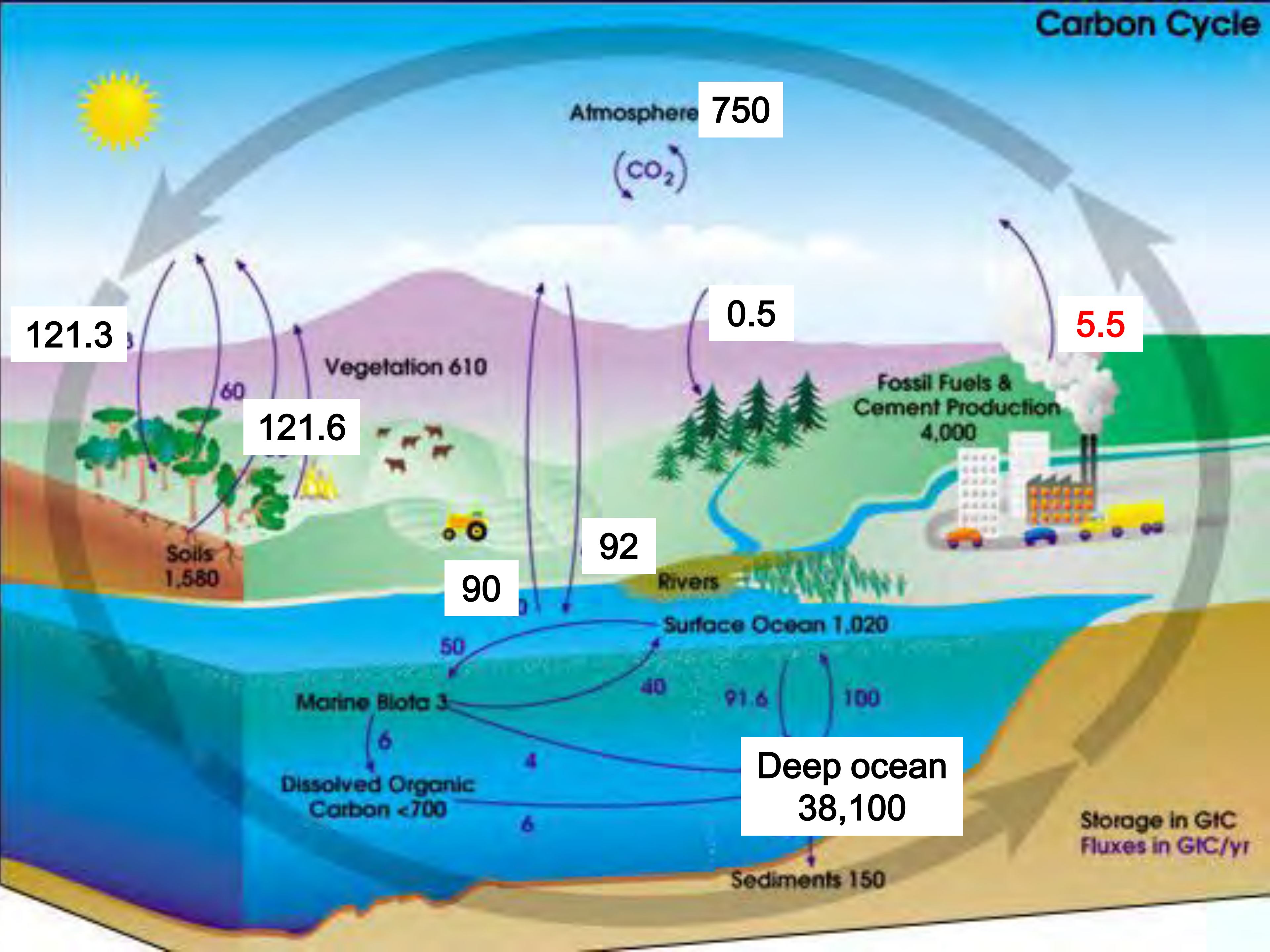
Computational Challenges of Climate Modeling

1. How will the sea level, sea-ice coverage, and ocean circulation change as the climate changes?

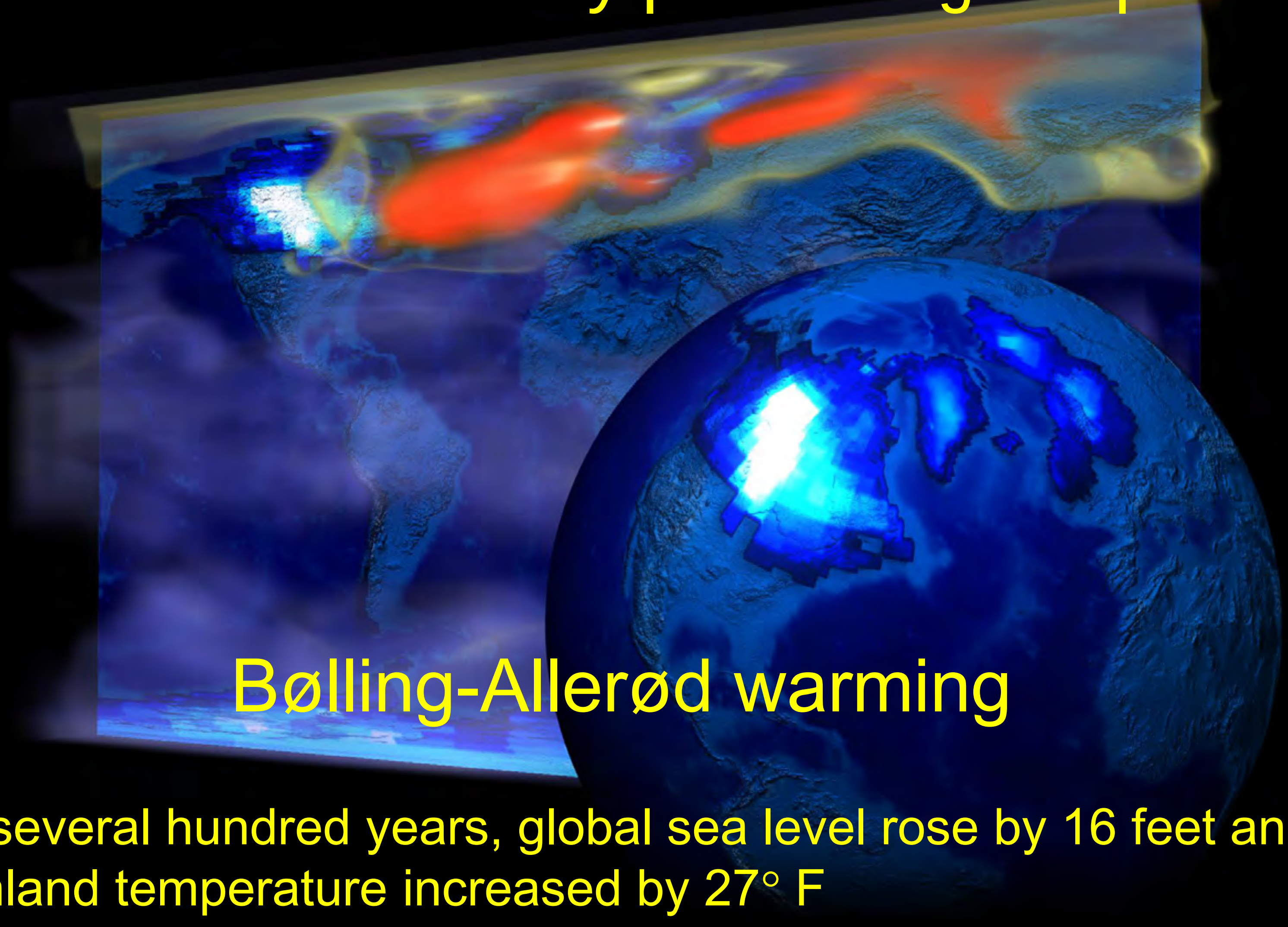
2. How will the distribution and cycling of water, ice, and clouds change with global warming?

3. How will extreme weather and climate change on the local and regional scales?

4. How do the carbon, methane, and nitrogen cycles interact with climate change?


Carbon Cycle
Atmosphere 750
CO2
121.3
60
121.6
Vegetation 610
0.5
5.5
Fossil Fuels &
Cement Production
4,000
Soils
1,580
92
90
Rivers
Surface Ocean 1,020
50
40
91.6
100
Marine Biota 3
6
4
Dissolved Organic
Carbon <700
6
Deep ocean
38,100
Sediments 150
Storage in GtC
Fluxes in GtC/yr

Validate models by predicting the past



Bølling-Allerød warming

Over several hundred years, global sea level rose by 16 feet and Greenland temperature increased by 27° F

- CO_2 increase of ~40 ppm
- Strengthening of the Atlantic Ocean's conveyor belt circulation
- Release of heat stored in the ocean over thousands of years

How is High Performance Computing changing Science and Technology?

1. Climate modeling and prediction
2. Industrial and building design

Computer design reduces development time

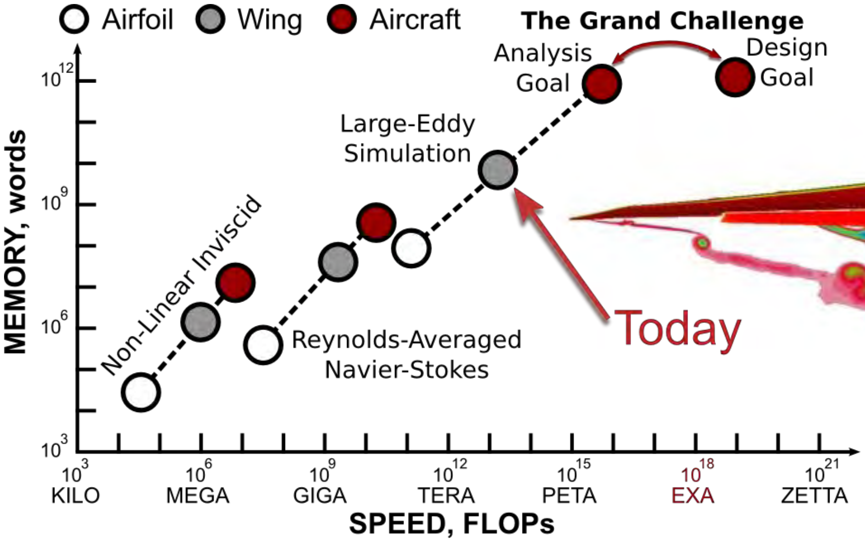
Cummins brought a diesel engine to market solely with computer modeling and analysis

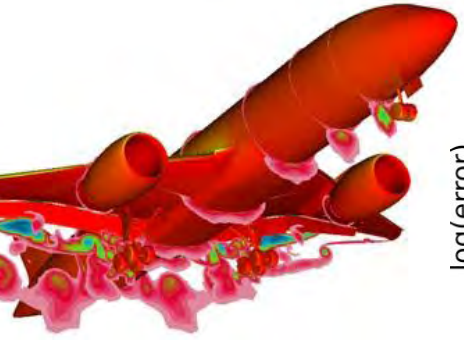
Reduction in development time and cost ~10 – 15%

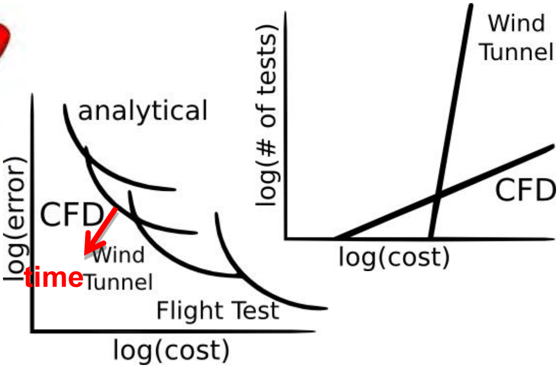
Goodyear tire designed with predictive modeling simulation tools

Factor of three reduction in product development time

The impact of High Performance Computing & Computational Fluid Dynamics on Boeing's Design Cycle







> ***"High Performance Computing has Fundamentally changed the way that Boeing designs flight vehicles."***
>
> **-Director, Boeing Commercial Airplanes**

1980 state of the art

Modern close coupled nacelle installation, 0.02 Mach faster than 737-200

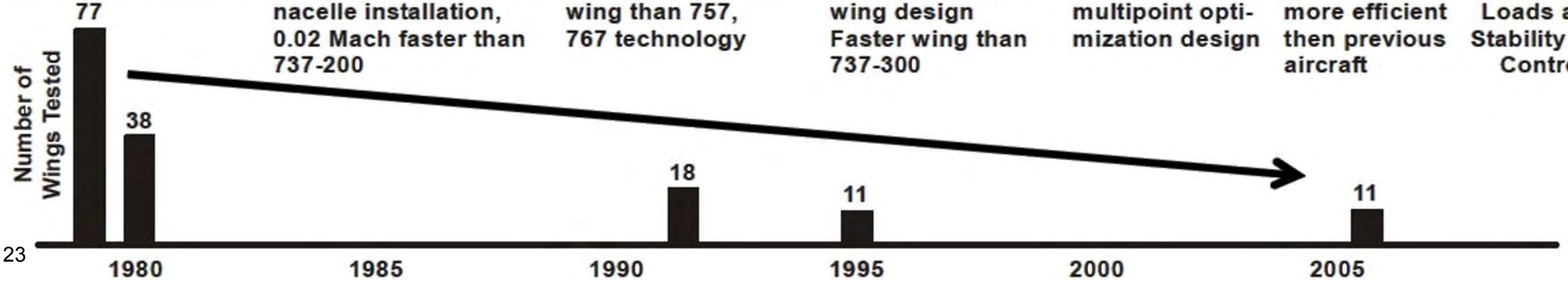
21% thicker faster wing than 757, 767 technology

Highly constrained wing design Faster wing than 737-300

Successful multipoint optimization design

Faster and more efficient then previous aircraft

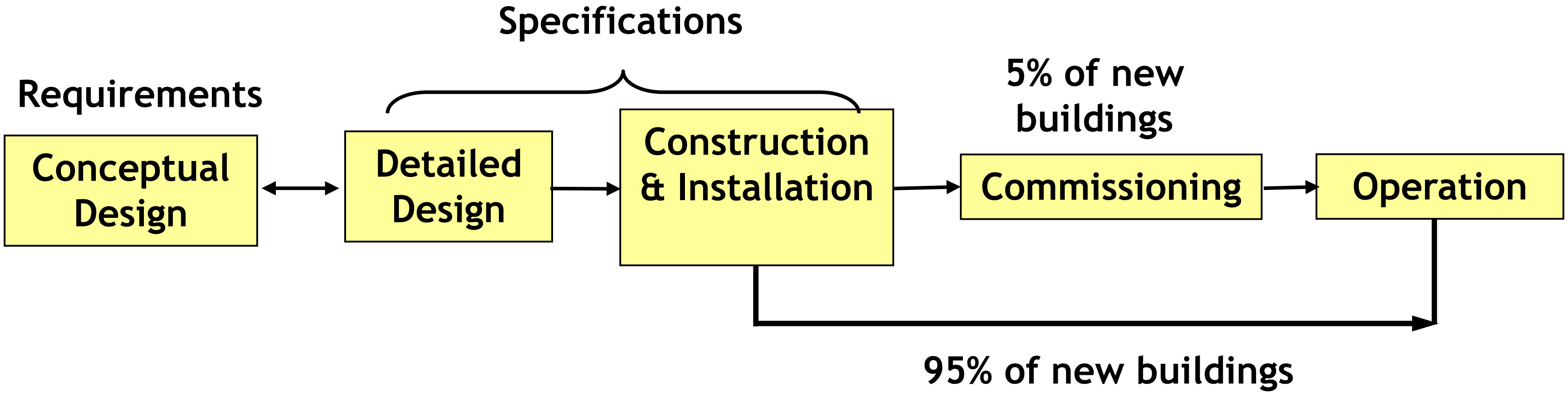
CFD for Loads and Stability and Control



Computation in Building Design

Buildings use about 40 percent of total U.S. energy

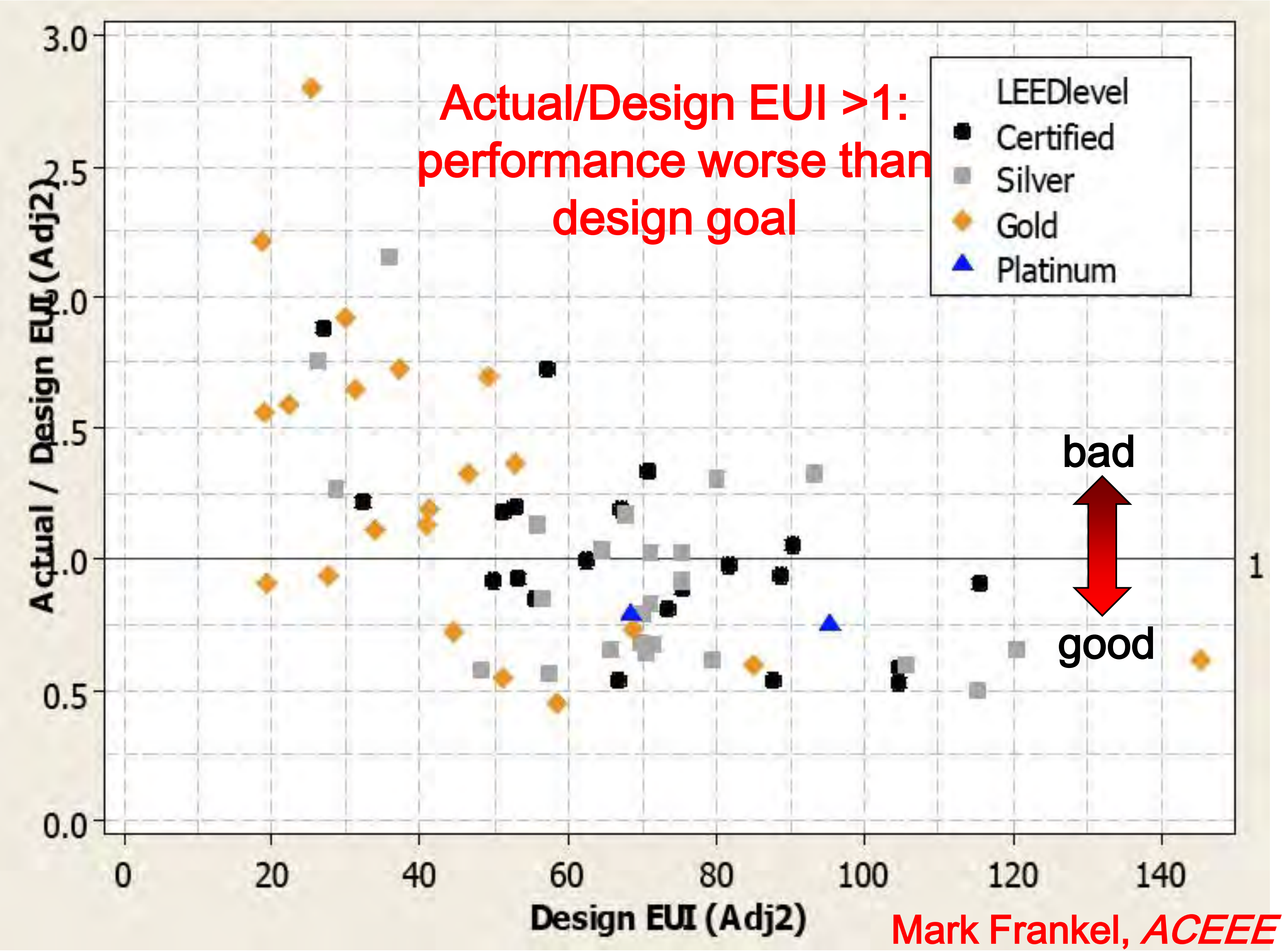
Current State:



United Technologies Analysis of lost energy efficiencies:

- 50% - Decisions in conceptual and detailed design (siting, facades, passive systems)
- 30% - Changes during construction & value engineering
- 20% - Monitoring of equipment and subsystem operations

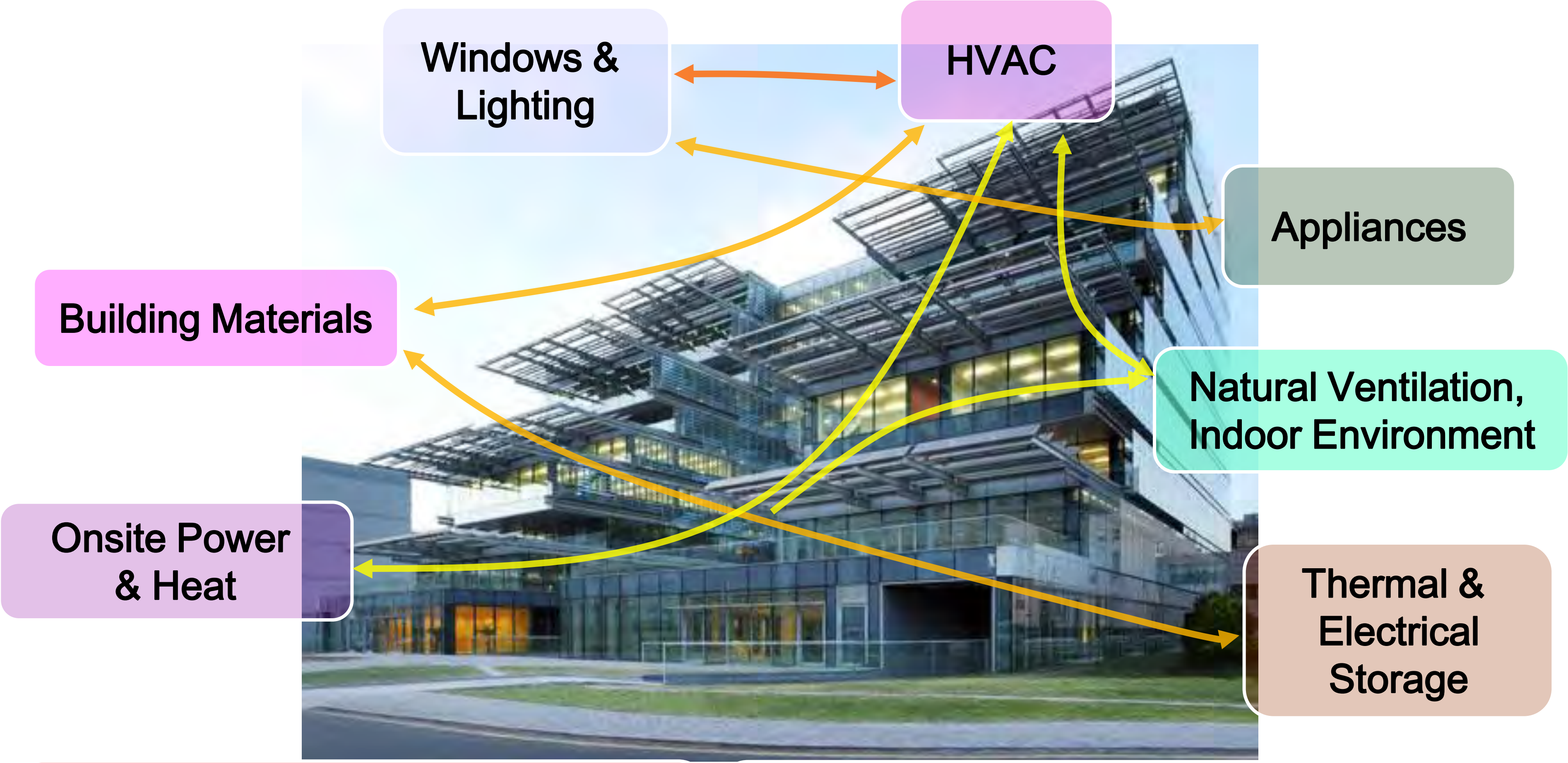
LEED ratings are based on design performance, not actual performance (EUI = End Use Intensity)



Actual/Design EUI >1: performance worse than design goal

Mark Frankel, *ACEEE* (2008)

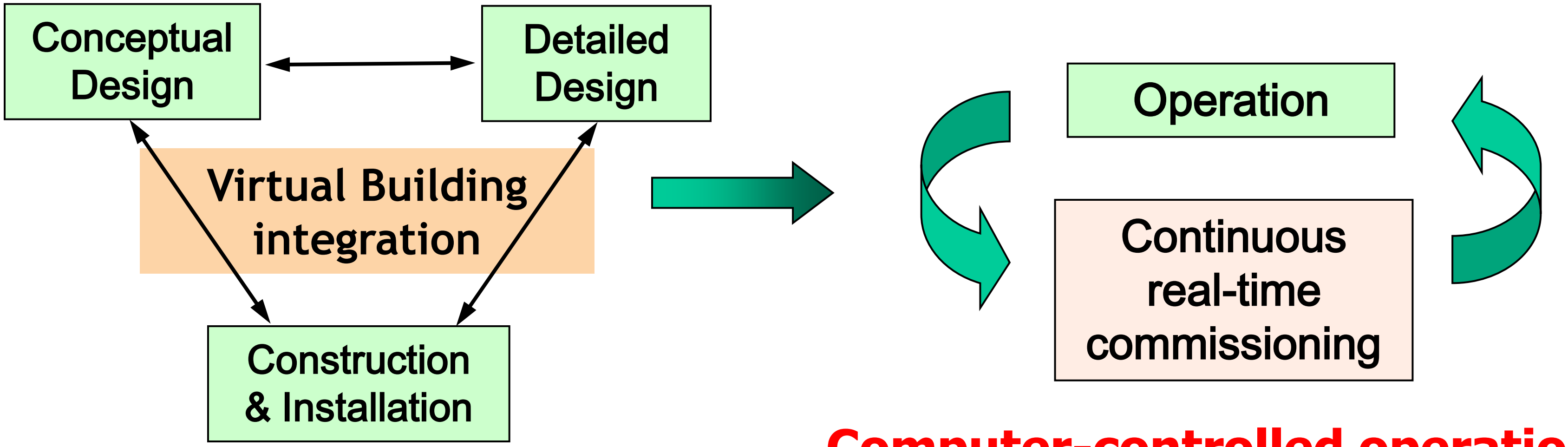
An understanding of the interfaces between all building sub-systems is needed for maximum energy efficiency



Building SPICE:
Tools to Design New Buildings
With Embedded Energy Analysis

Building Operating Platform (BOP)
Sensors, Communication, Controls,
Real-Time Optimization

A new way of designing and constructing buildings.



Conceptual Design

Detailed Design

Virtual Building integration

Construction & Installation

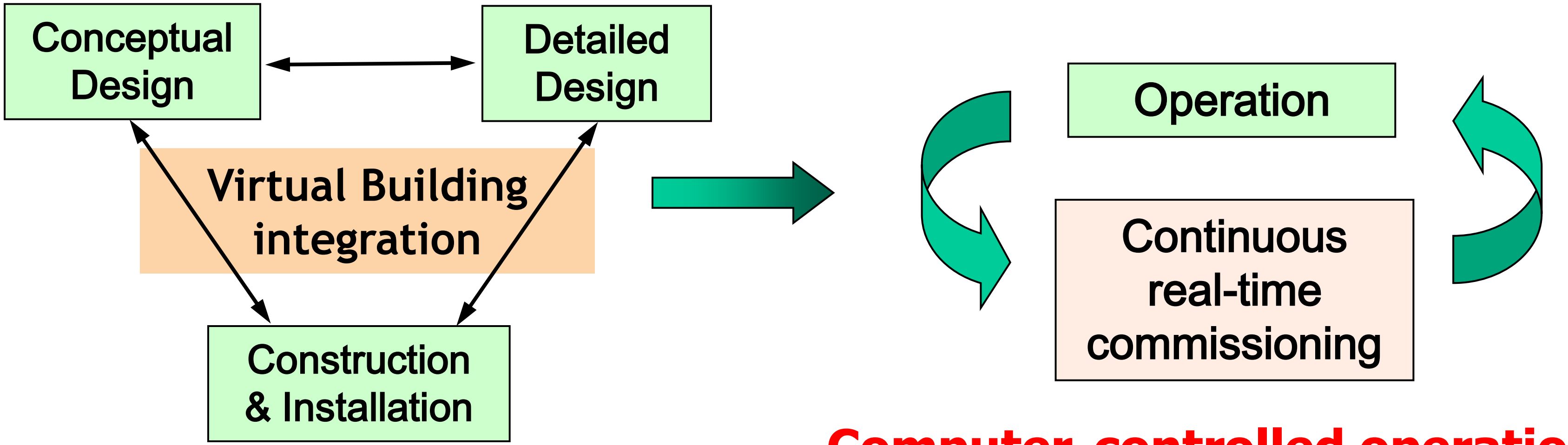
Operation

Continuous real-time commissioning

Computer-aided design tools with Embedded Energy Analysis

Computer-controlled operation with Sensors and Controls for Real-Time Optimization

A new way of designing and constructing buildings.



Conceptual Design

Detailed Design

Virtual Building integration

Construction & Installation

Operation

Continuous real-time commissioning

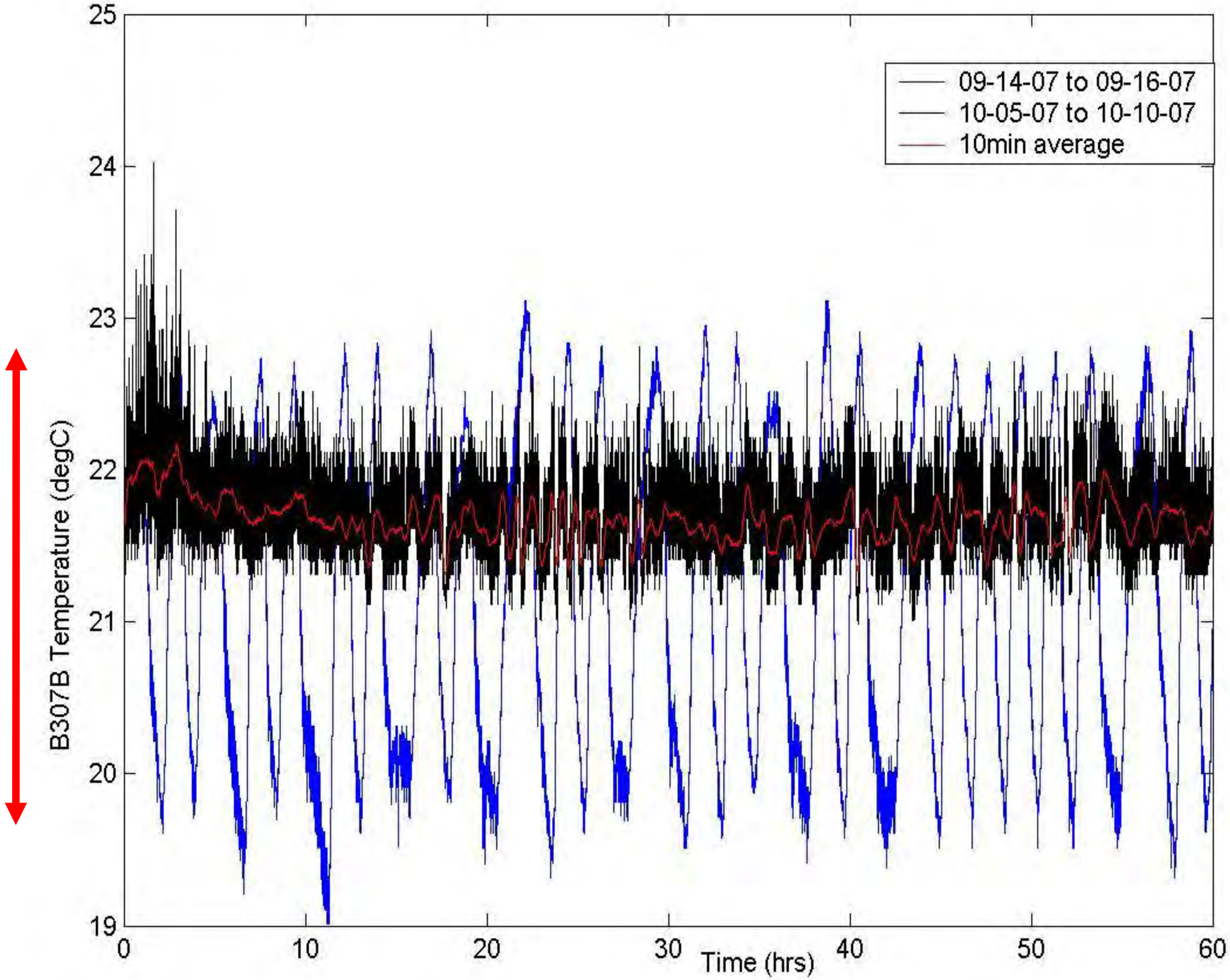
Computer-aided design tools with Embedded Energy Analysis

Computer-controlled operation with Sensors and Controls for Real-Time Optimization

- Oxygen sensor
- Air pressure sensor
- Air temperature sensor
- Engine temp. sensor
- Throttle position sensor
- Knock sensor

U.C. Berkeley: New Stanley Hall
$162 M multidisciplinary building

Temperature oscillations measured in the Chu Lab microscope room



Temperature variation > 3°C

Reduced to < 0.3 °C

Buildings are a complex, multi-scale dynamical system requiring distributed sensing, control and optimization.

- **Computer tools** must enable preliminary and detailed design cycle times in the order of a few weeks,

- Produce accurate high fidelity simulations of the designed building with control systems operating in closed loop,

- Develop a hierarchical controller design framework that provides controllers for multi-scale in time and space systems.

From a 2007 White Paper on the "*Development of Computational Methods & Tools for Design, Optimization and Control of Energy Efficient Buildings*," John Burns , Clas Jacobson, Satish Narayanan, et al.

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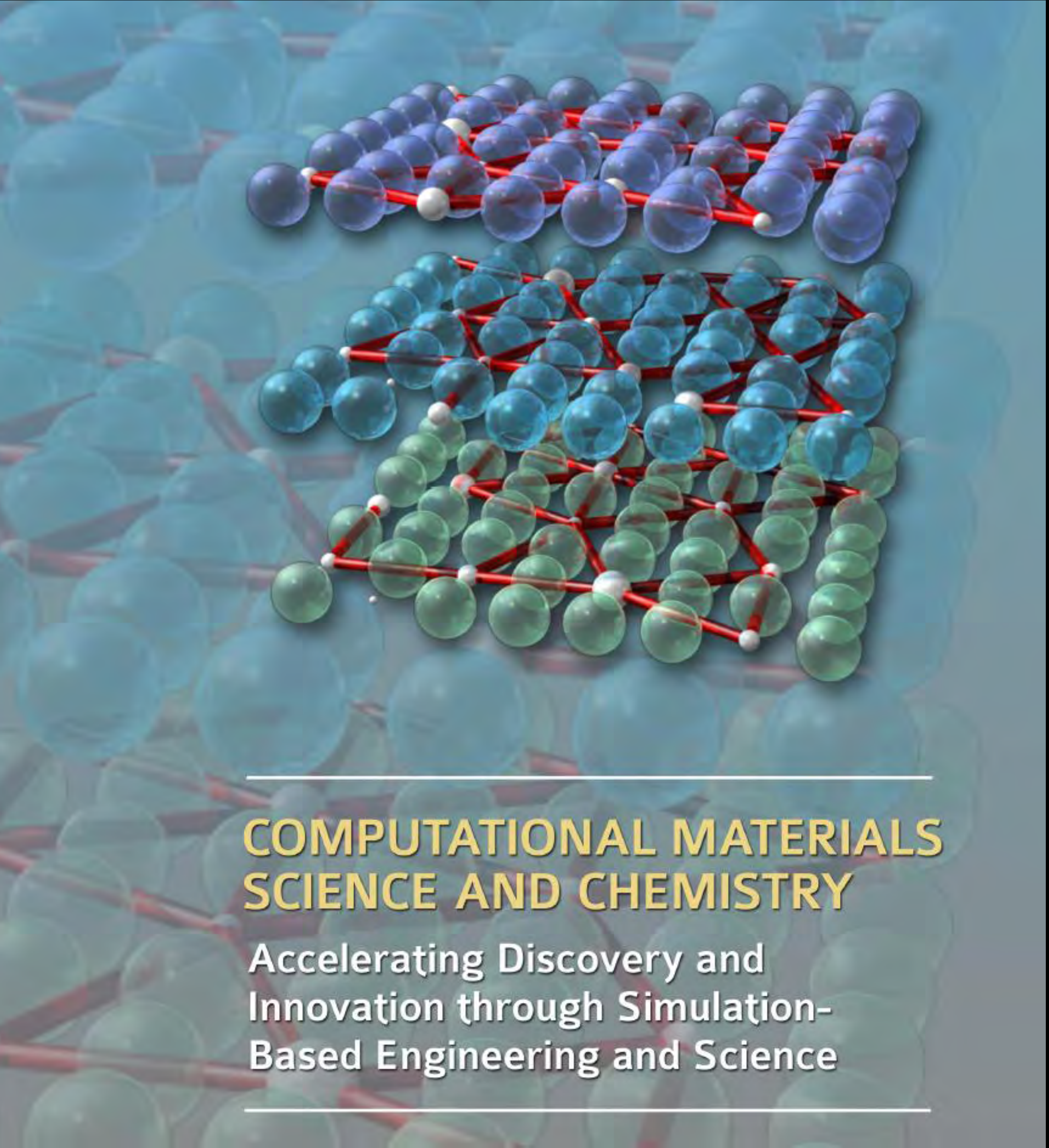


COMPUTATIONAL MATERIALS
SCIENCE AND CHEMISTRY

Accelerating Discovery and
Innovation through Simulation-
Based Engineering and Science

DOE workshop

July 26–27, 2010

Last week, the Office of Science released a report on accelerating innovation through simulations and HPC

"For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled. This ability is ***transformational*** *for the discovery process."*

Transformative materials…

- Materials for extreme conditions
- Light harvesting materials
- Materials designed at the nano-scale catalysts
- Strongly correlated systems

Stainless Steels with Higher-Temperature Capability Needed

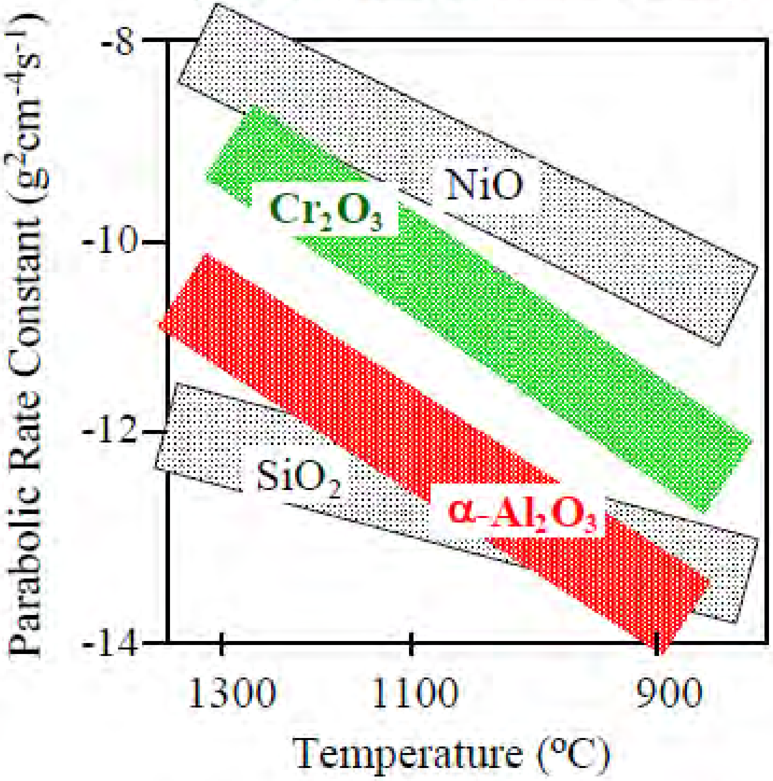
- Driver: Increased efficiencies with higher operating temperatures in power generation systems.

- Key issues are creep and oxidation resistance.

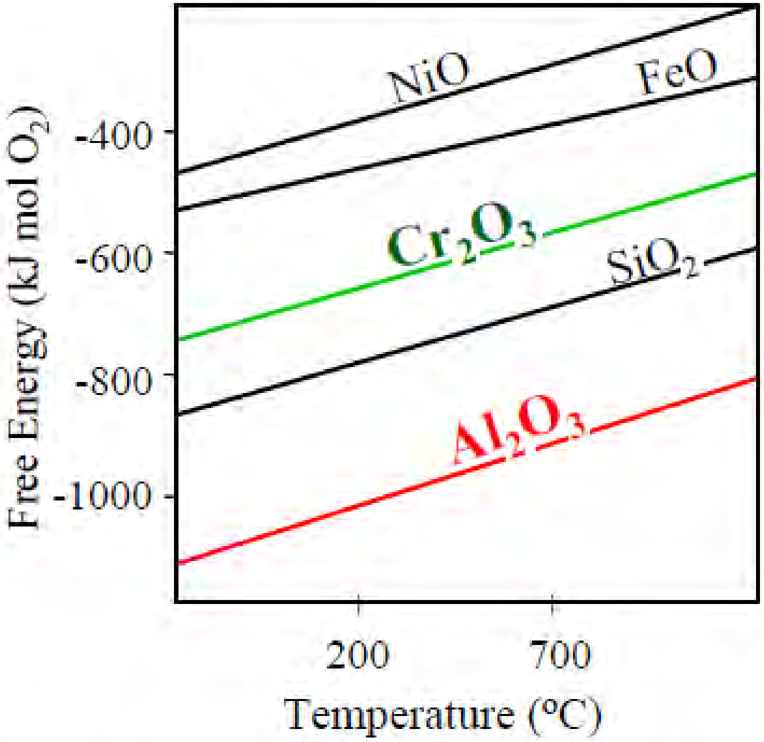
  - Significant gains have been made in recent years for improved creep resistance via nano MX precipitate control (M = Nb, Ti, V; X = C, N).

  - Stainless steels rely on Cr_2O_3 scales for protection from high-temperature oxidation.
    -Limited in many industrial environments (water vapor, C, S)
    -Most frequent solution is coating: costly, not always feasible

Al_2O_3 Scales Offer Superior Protection in Many Industrially-Relevant Environments



=Kinetics=
(Growth rate of oxide scales)

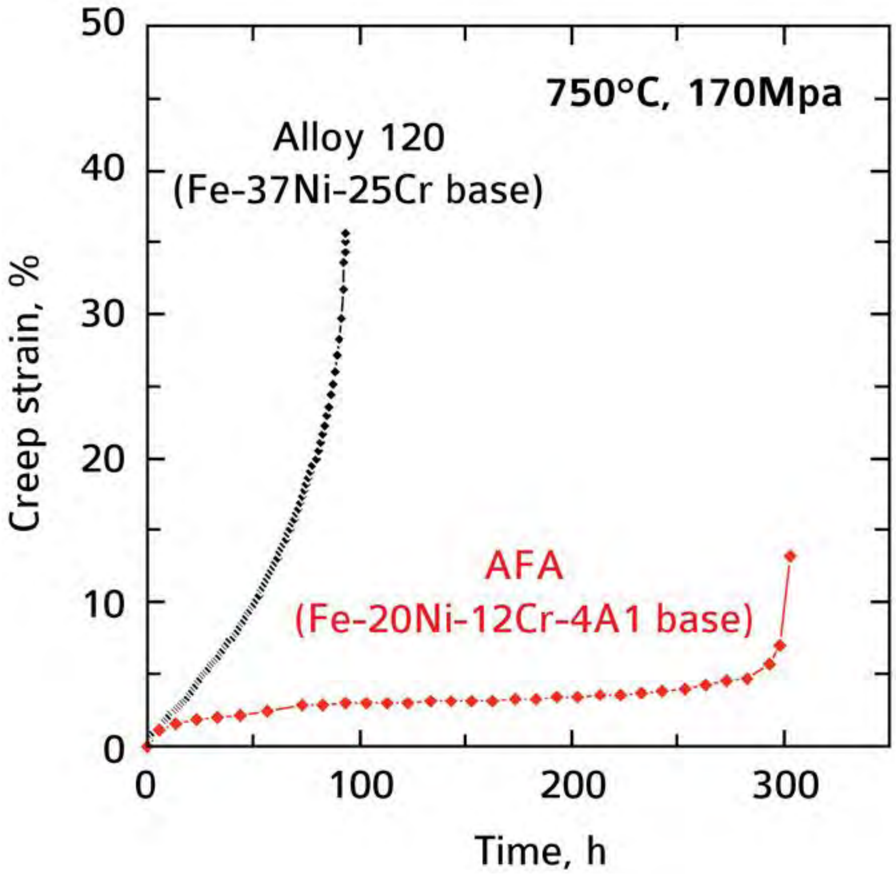


=Thermodynamics=
(Ellingham diagram)

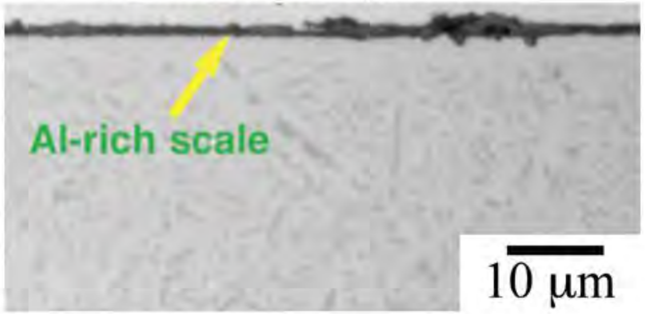
- Al_2O_3 exhibits a lower growth rate and is more thermodynamically stable in oxygen than Cr_2O_3.
- Highly stable in water vapor.

Computational techniques enabled the rapid development of alumina-forming austenitic (AFA) stainless steels

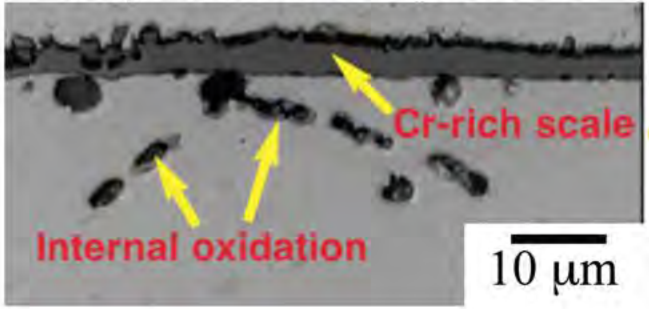
- Protective alumina scale formation (10x improvement)
- High creep resistance from stable nano-scale MC carbides and inter-metallic precipitates.
- Low cost



AFA 800°C 10,000 h Air

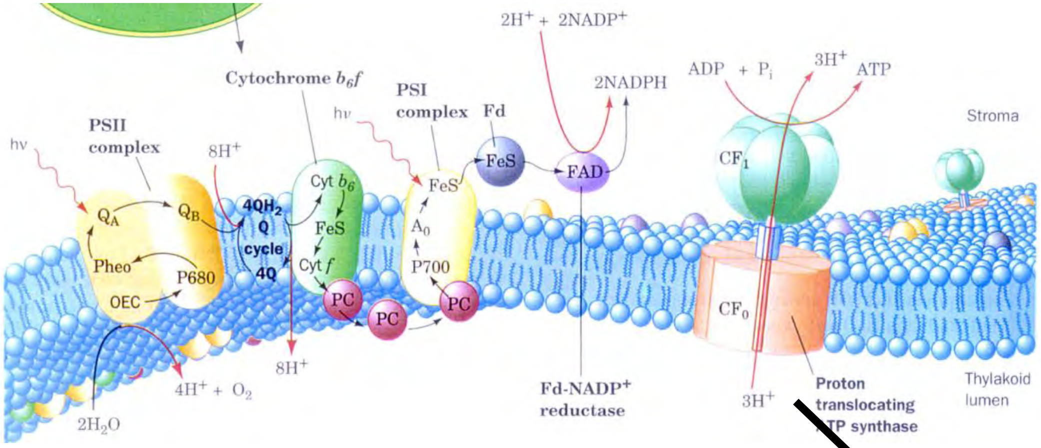


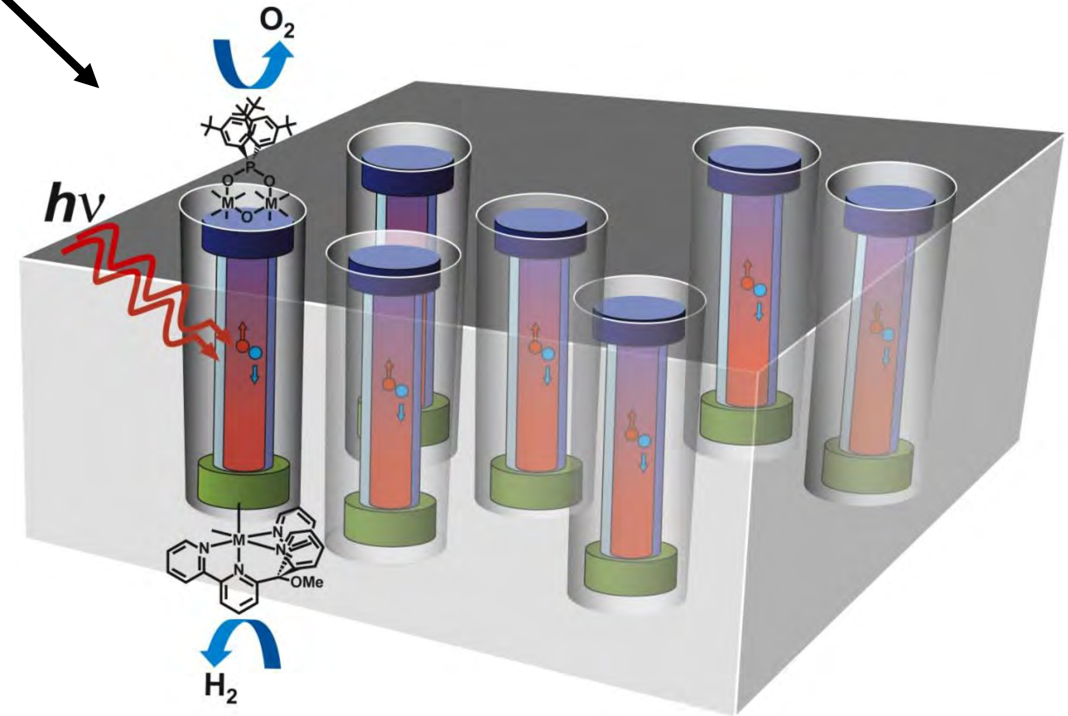
Alloy 120 800°C 10,000 h Air



Man first learned to fly by imitating nature

Artificial Photosynthesis?



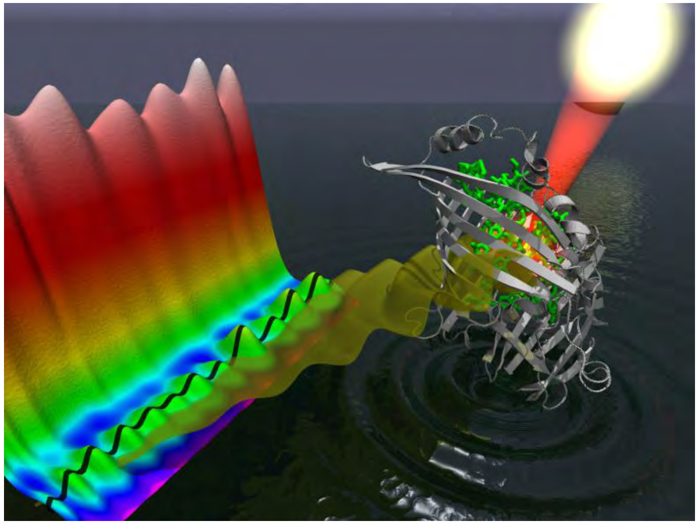


The first important step is to use sunlight to “split” water into oxygen and hydrogen.

HPC for photosynthesis

Quantum Effects in Photosynthesis

- **Photosynthetic complexes can be up to 98% efficient via the interplay of quantum and classical effects**
- **Electronic quantum coherence driving the efficiency of photosynthesis**



Joint Center for Artificial Photosynthesis

Cal Tech and LBNL awarded DOE Energy Innovation Hub

CALTECH

JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

BERKELEY LAB

- **Requesting 20M CPU hrs/year to ramp to 35M CPU hrs/year by year 4**
  - **Catalysis**
  - **Nano-fluidics**
  - **Light absorption and charge dynamics**
  - **Nano-photovoltaics**

“Is Life Based on the Laws of Physics? “

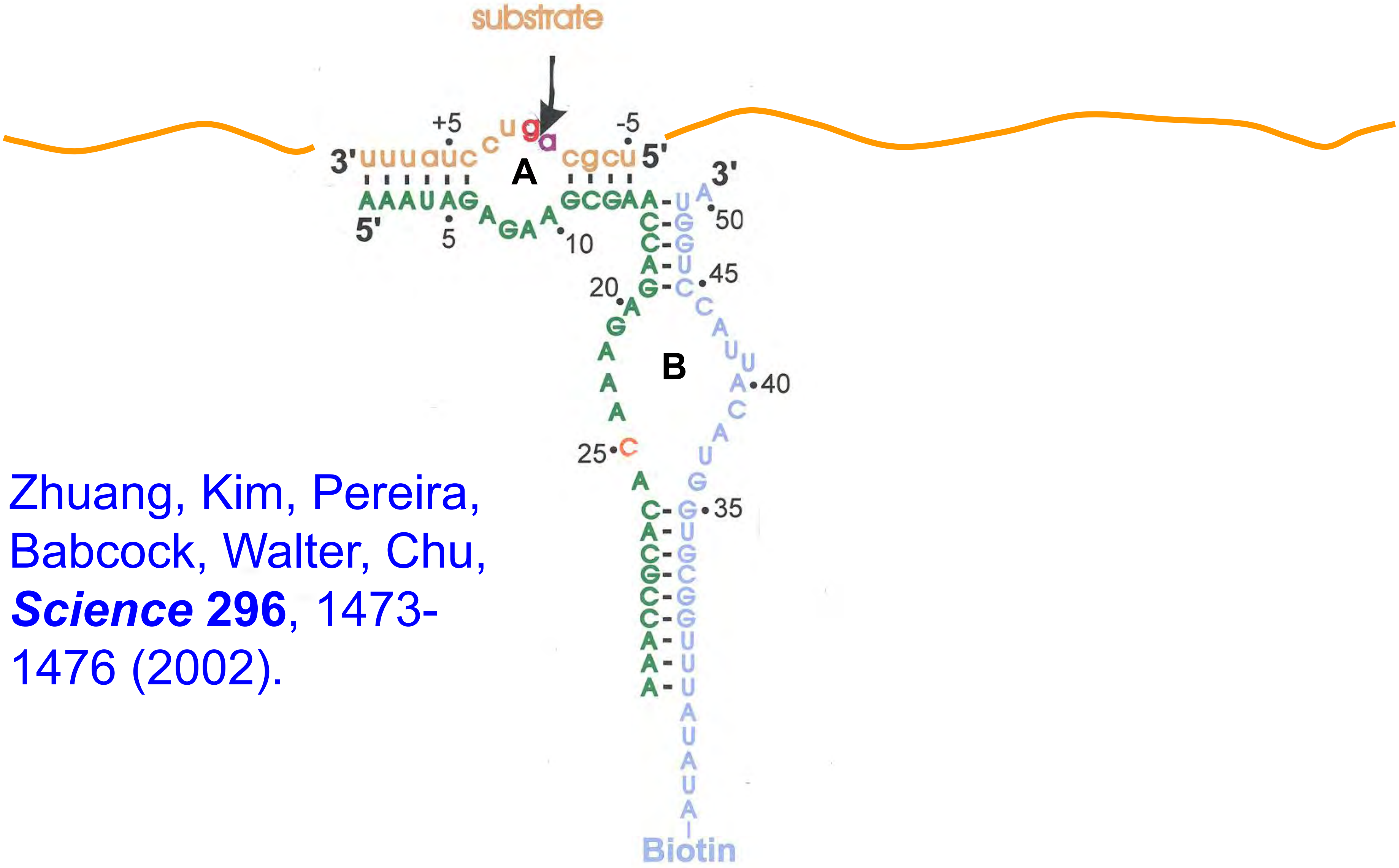
“…from all we have learnt about the structure of living matter, we must be prepared to find it working in a manner that **cannot** be reduced to the ordinary laws of physics … but because the construction is different from anything we have yet tested in the physical laboratory.

Erwin Schrödinger, 1944

Man-made machines work where **friction** is minimized.

In an organism, the molecular machinery is imbedded in a viscous fluid. Friction and thermal fluctuations are huge.

Hairpin Ribozyme: an example of how nature uses new design rules at the molecular scale



Zhuang, Kim, Pereira, Babcock, Walter, Chu, ***Science* 296**, 1473-1476 (2002).

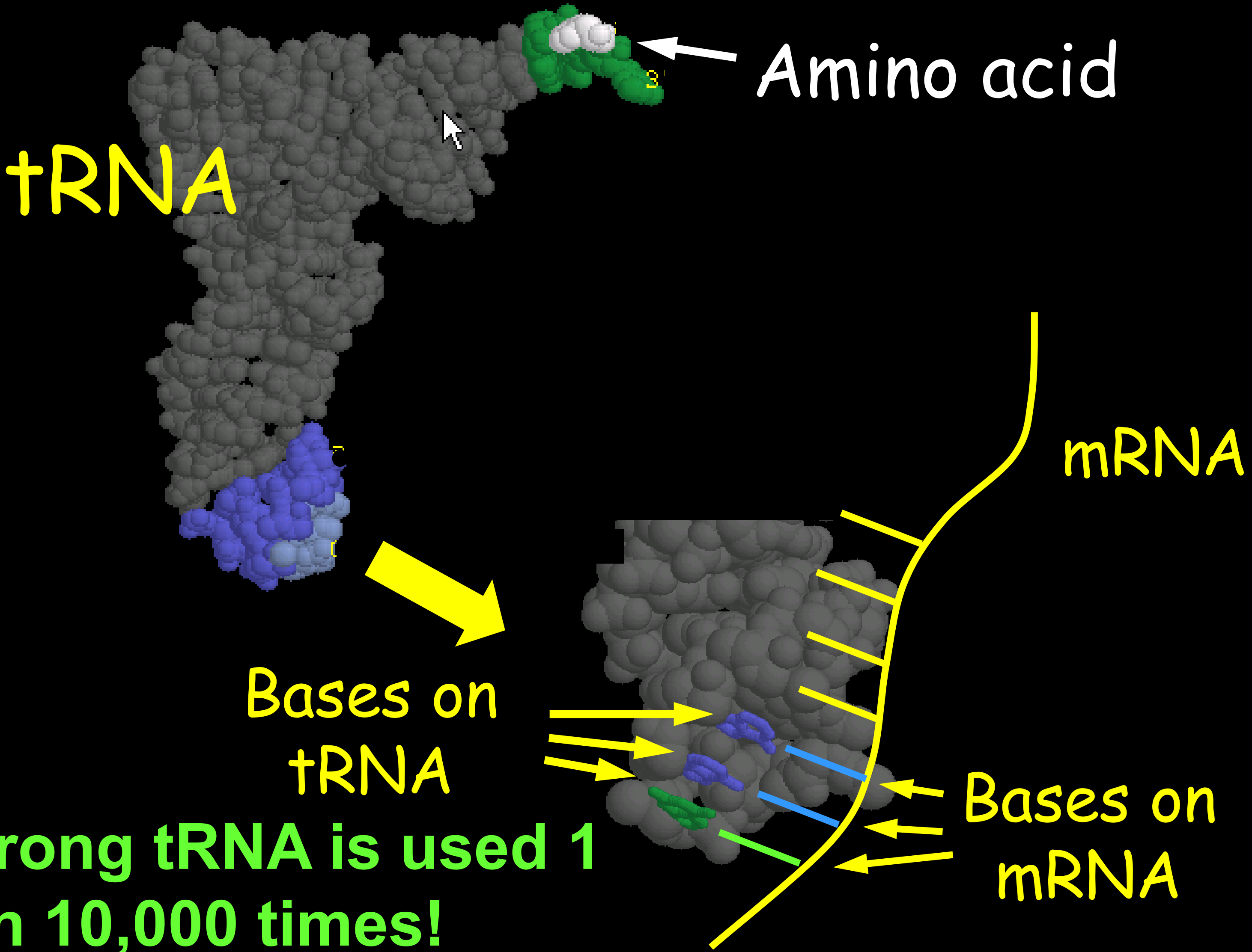
The Ribosome

Thermal fluctuations of t-RNA in the ribosome play a critical role in the selection fidelity

Ribosomal Proteins are located on the Periphery of the Ribosome

20 nm

Each amino acid is brought into the ribosome by transfer RNA (tRNA)



Amino acid

tRNA

mRNA

Bases on tRNA

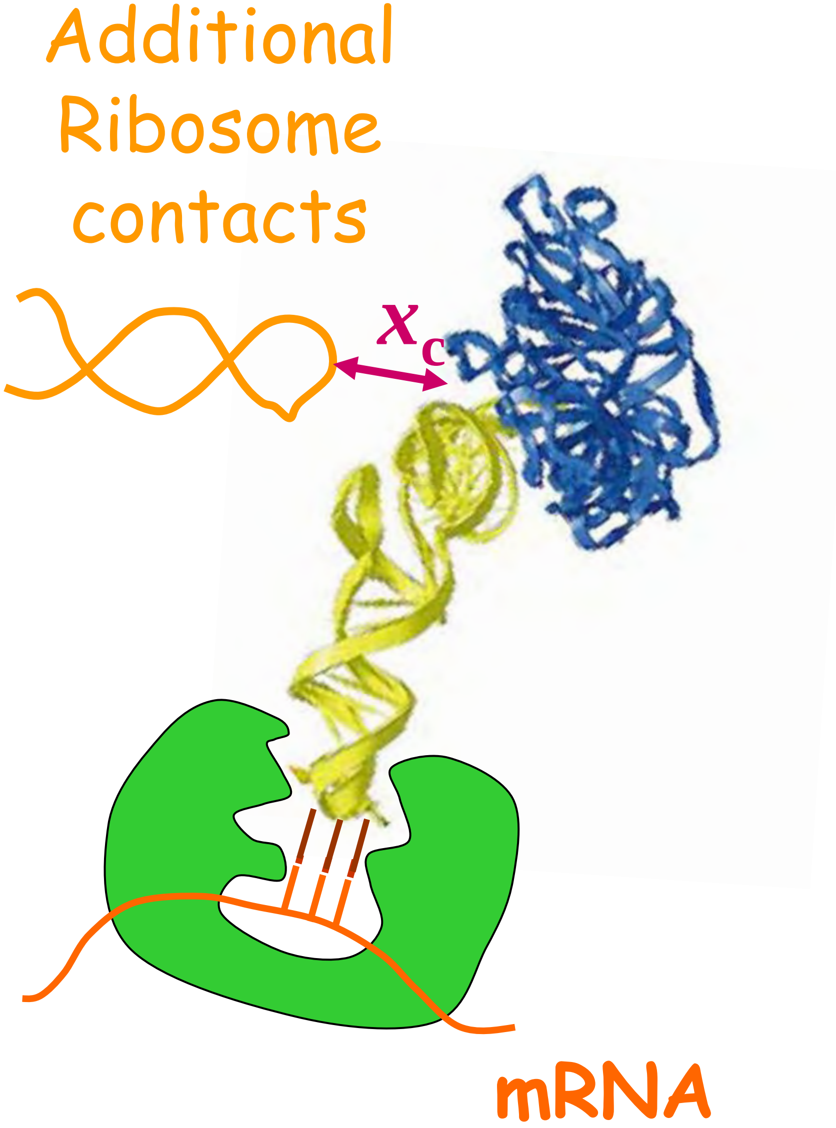
Bases on mRNA

The wrong tRNA is used 1 in 10,000 times!

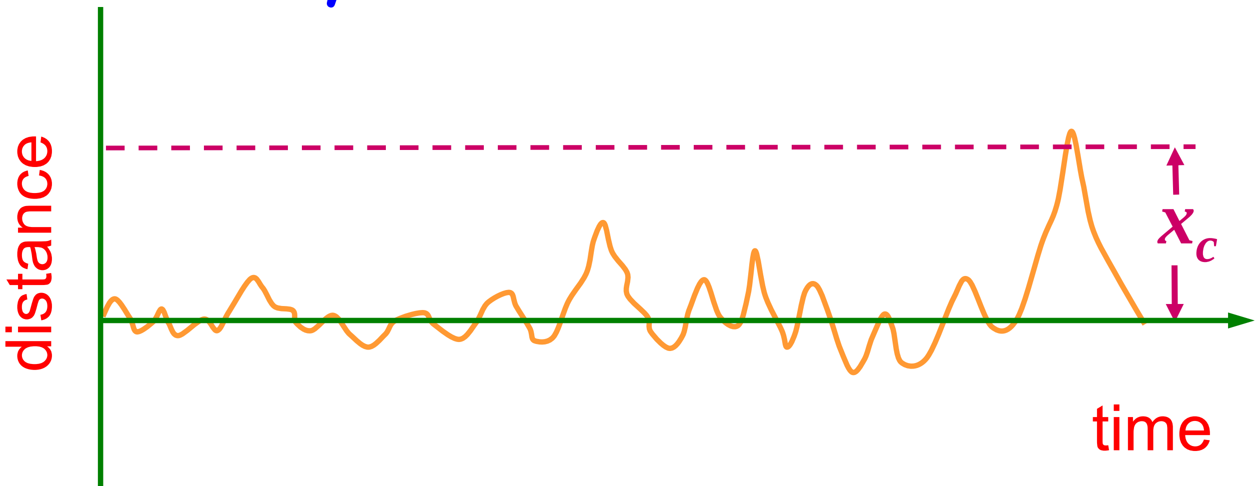
Our proposed selection mechanism

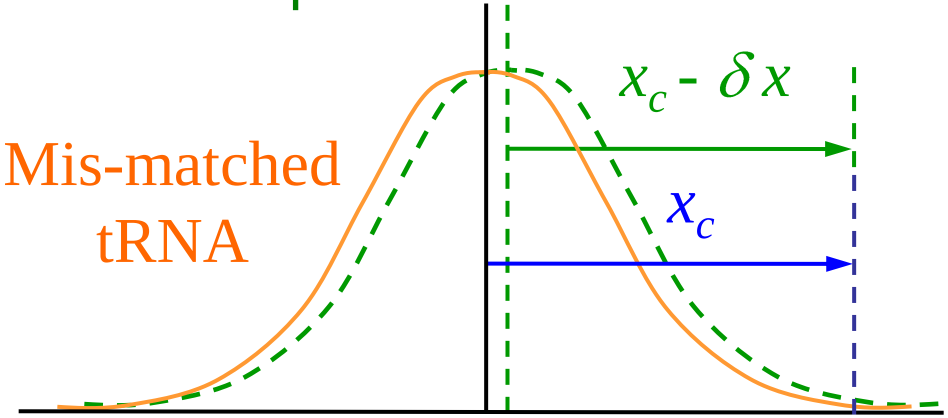
1) Proper base-paring causes the ribosome to wrap around the base of the tRNA

2) The wrapping of the ribosome causes the tRNA to move into a position so it is more likely to make stabilizing contacts with the Ribosome.



If you were the design engineer, how would you make the ribosome?





$$\frac{\nu e^{-(x_c-\delta x)^2/\sigma^2}}{\nu e^{-x_c{}^2/\sigma^2}} \approx e^{+2x_c\delta x/\sigma^2}$$

Understanding correlated electron systems

Richard Feynman:

“The force on any nucleus (considered fixed) in any system of nuclei and electrons is just the classical electrostatic attraction exerted on the nucleus in question by the other nuclei and by the electron charge density distribution for all electrons.”

How does one compute the electron charge density using the laws of quantum mechanics?

Jacob’s Ladder to chemistry heaven

Increasingly better calculation of electron correlation effects.

Computational cost increases by a factor of 10–100 going from the second and third rungs to the fourth rung.

Local Density Approximation

Zeroth-order electron-electron interactions

Simulation is now the "third leg" of Science

- Theory
- Simulation
- Experiment