Energy and Computational Science

Steven E. Koonin
Under Secretary of Energy for Science
August 2009

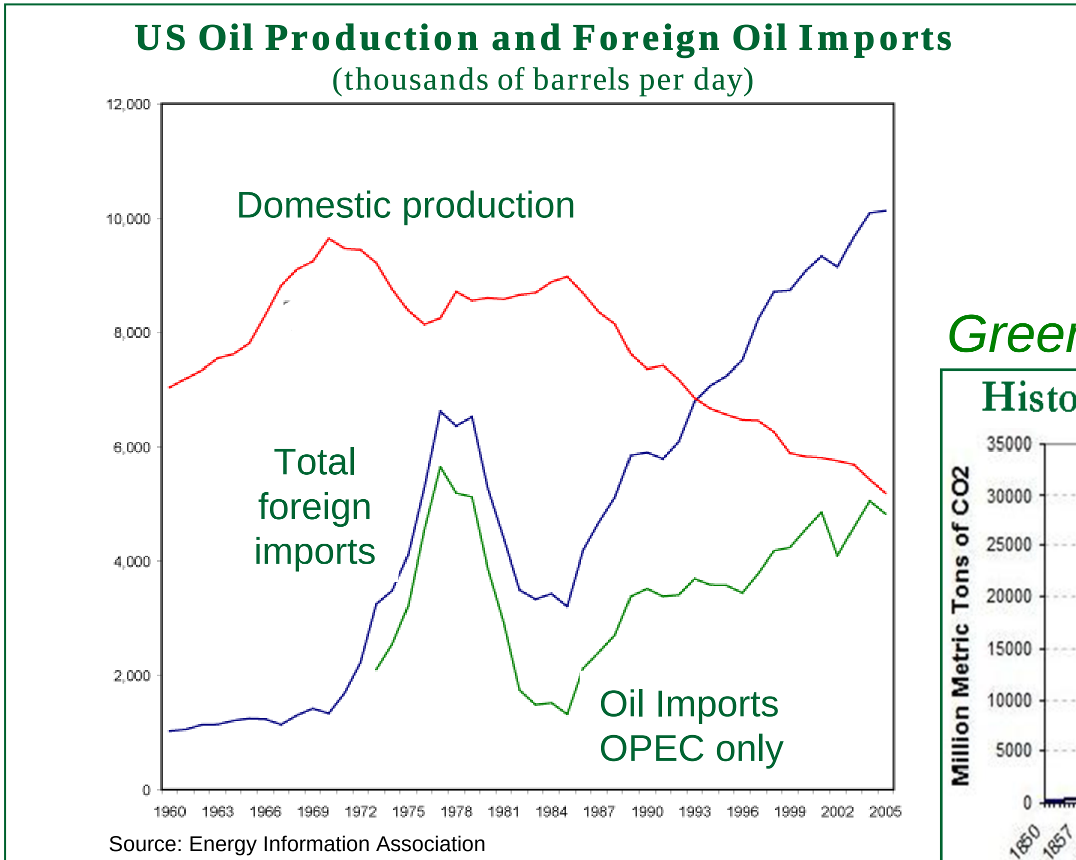
My roles at DOE

In many ways, it still looks like this…

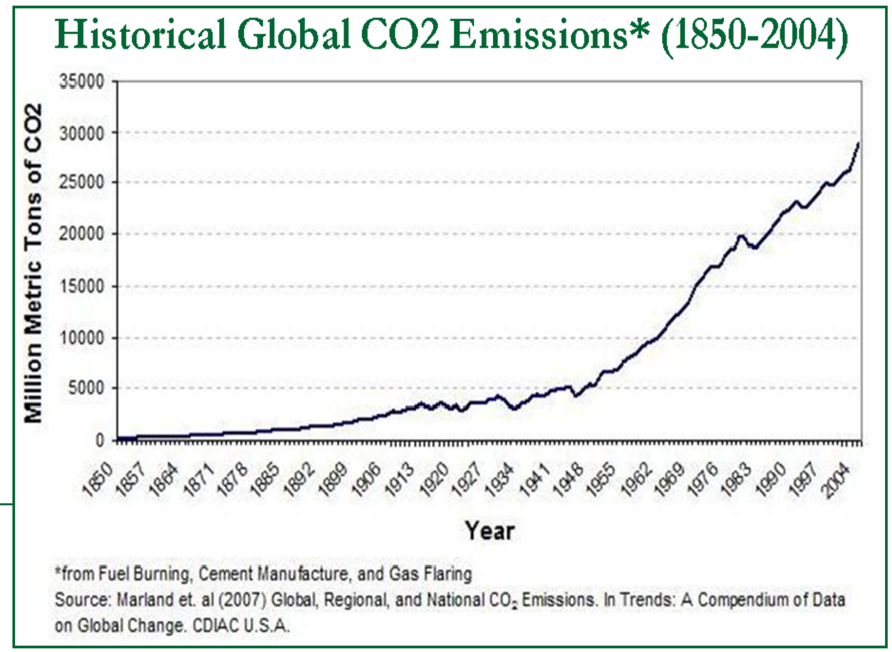
- Chief Scientist of the DOE (not the Director of SC)
- Enable cross disciplinary ideas and research to flourish
- Define and enable science programs that
  - Knit the department together and
  - Lead to novel energy research efforts

America's energy challenges

Security of Supply

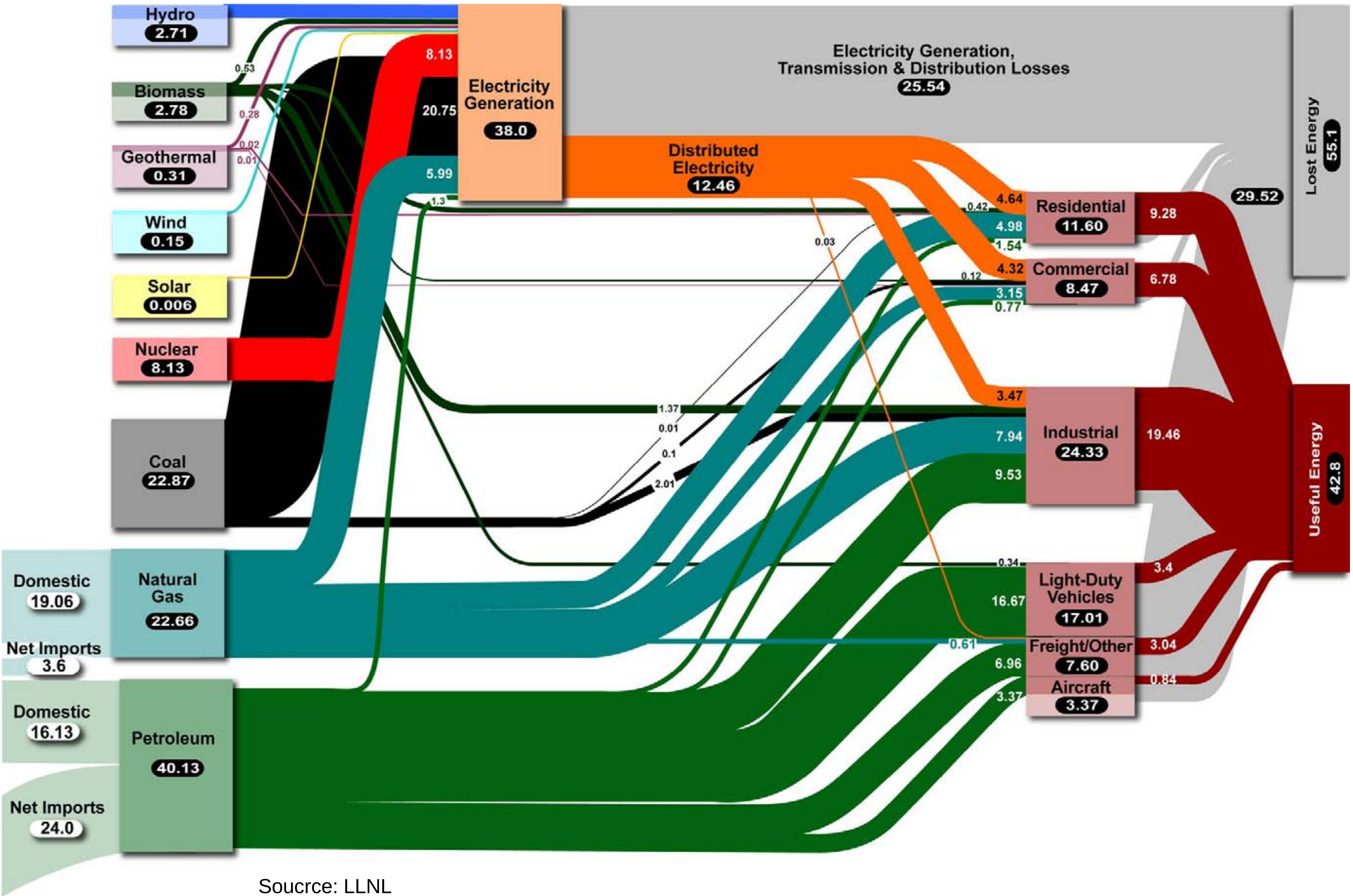


Greenhouse Gas Emissions



U.S. DEPARTMENT OF ENERGY

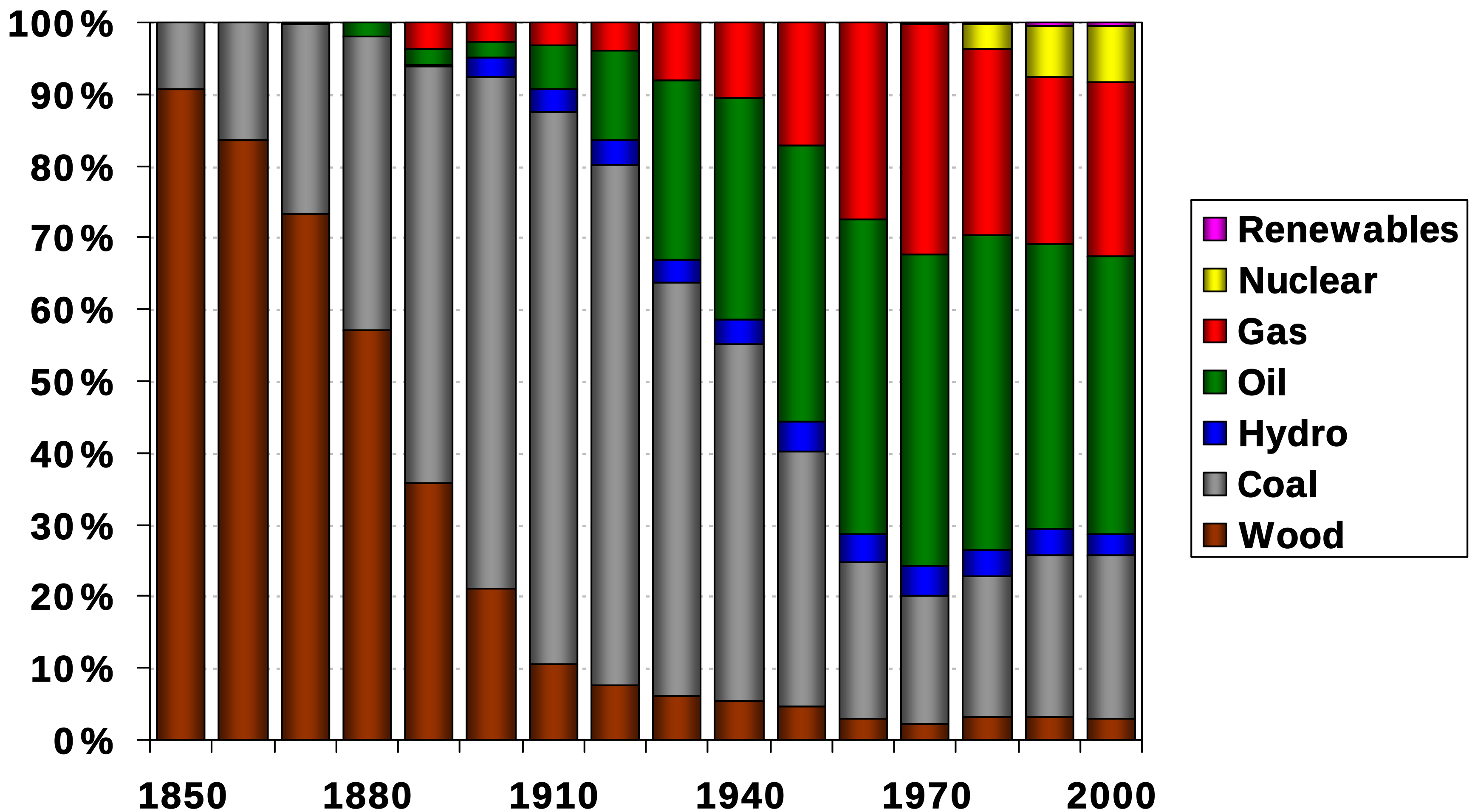
US Energy flows (~ 100 Ej annually)



Soucrce: LLNL

Energy technologies change slowly

US energy supply since 1850



Source: EIA

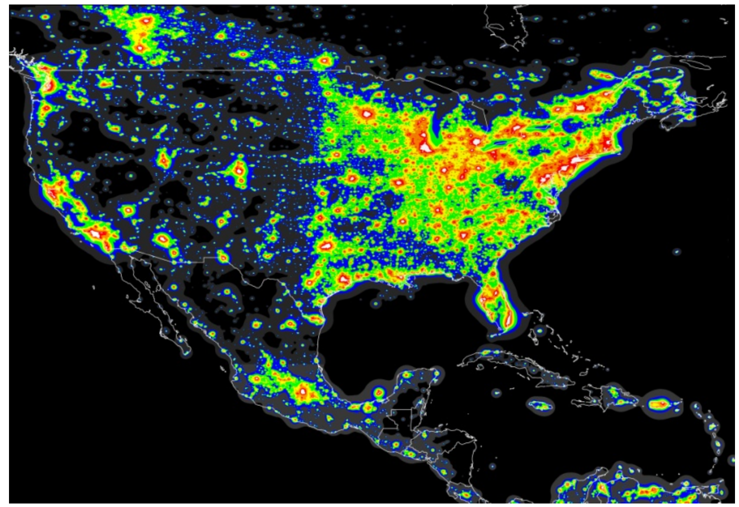
U.S. DEPARTMENT OF ENERGY

Why is energy different?

Scale

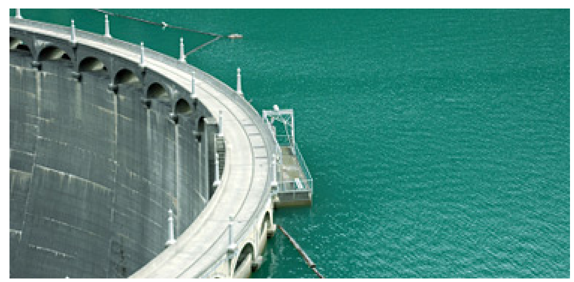
*Large **capital** and access to existing **infrastructure** are required*

Ubiquity *Consider **economic**, **political**, and **social** dimensions*



Incumbency

*Technology requires a **full-chain** effort*



Interoperability

*Transformation will take a **long time***

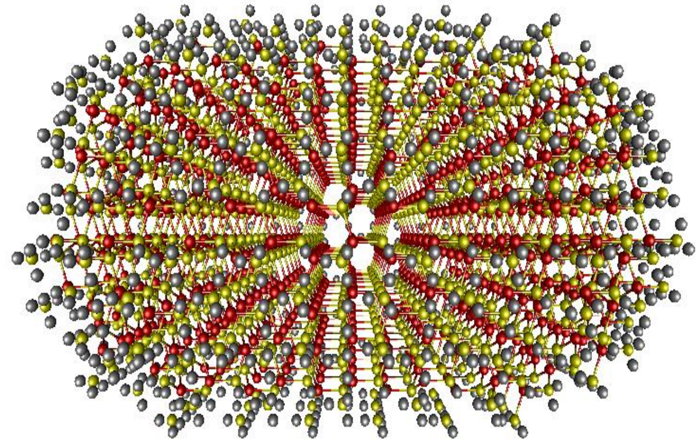
U.S. DEPARTMENT OF ENERGY

Energy relevant computation

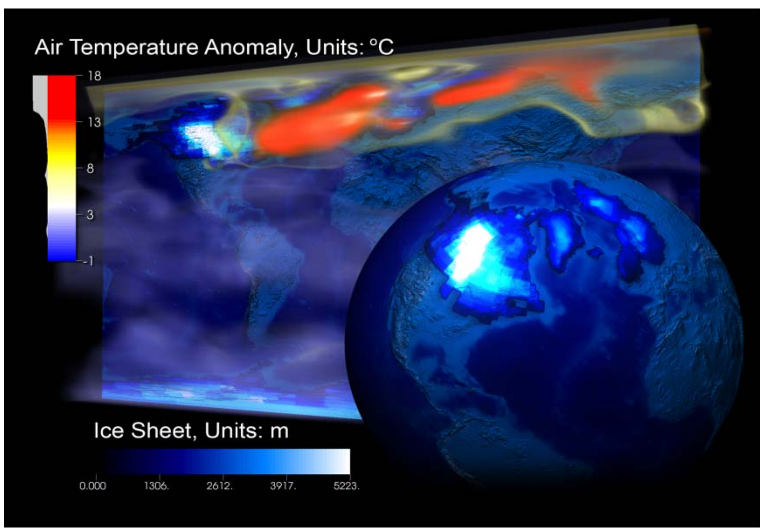
Novel divide & conquer approach to solve DFT by reducing $O(n^3)$ to $O(n)$

Design of new materials
for solar cells, Wang et al., SC08

$Cd_{961}Se_{724}H_{948}$



Dipole moment calculated on 2633 atom quantum rod



Simulations show deglaciation during the Bølling-Allerød, Earth's most recent period of natural global warming.
Featured in the July 17 issue of the journal Science

Computing for Nuclear Energy

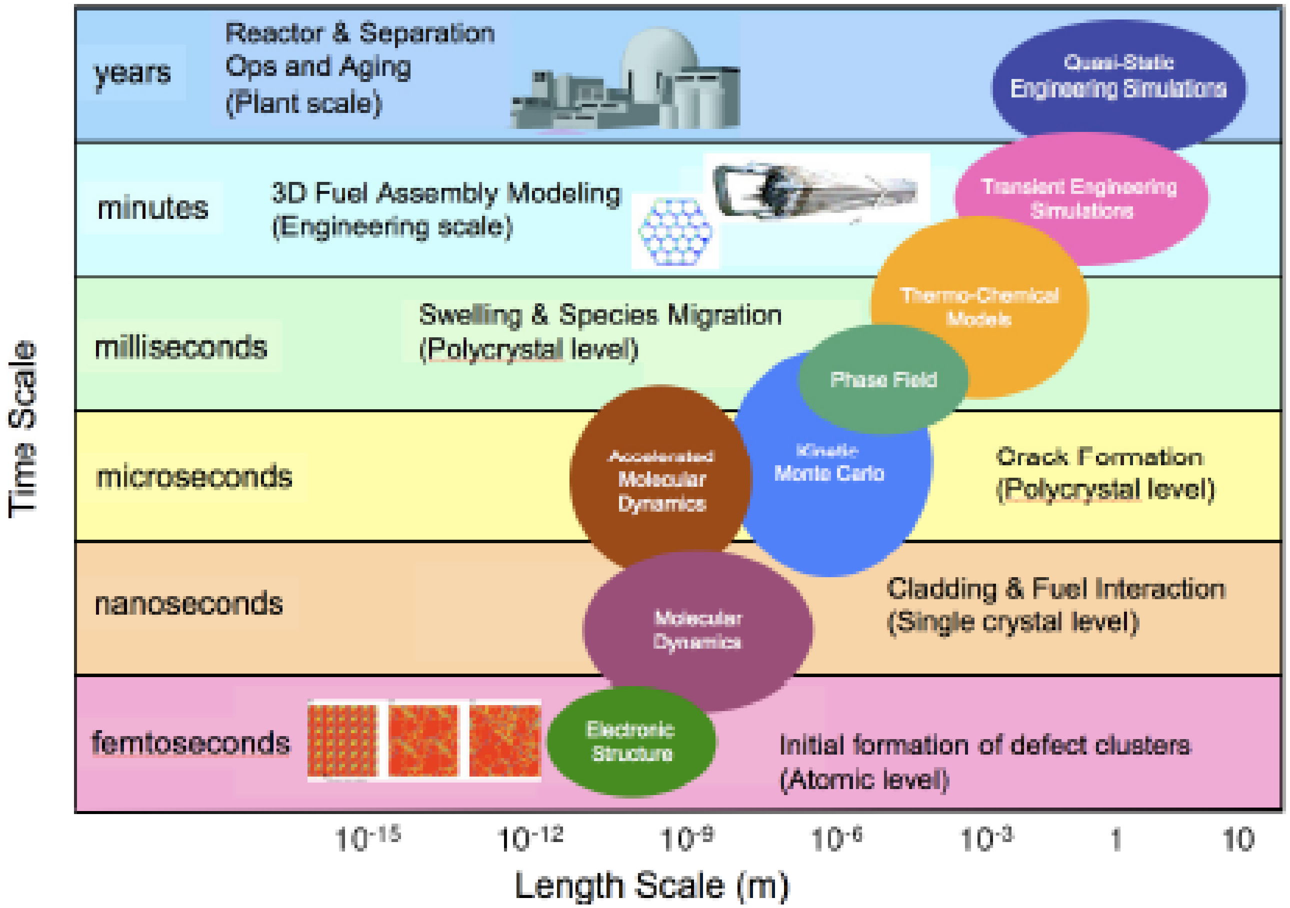


Figure 1. Multi-scale challenge.

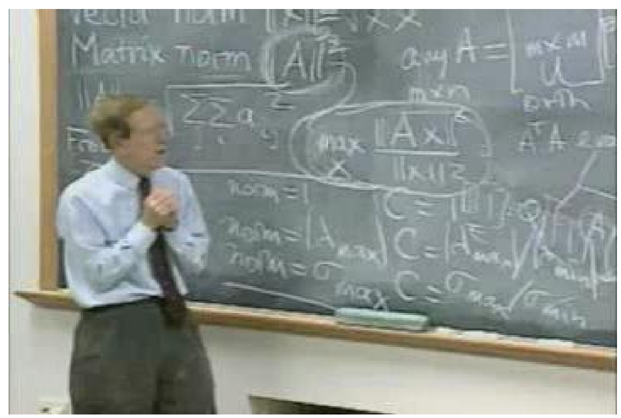
Multiple scales
Multiple physics
Systems approach required

Potentially significant impacts: reliability, safety, efficiency gains

From ASCAC/NE workshop on
Science based Nuclear Energy systems Enabled by
Advanced Modeling and Simulation at the Extreme Scale

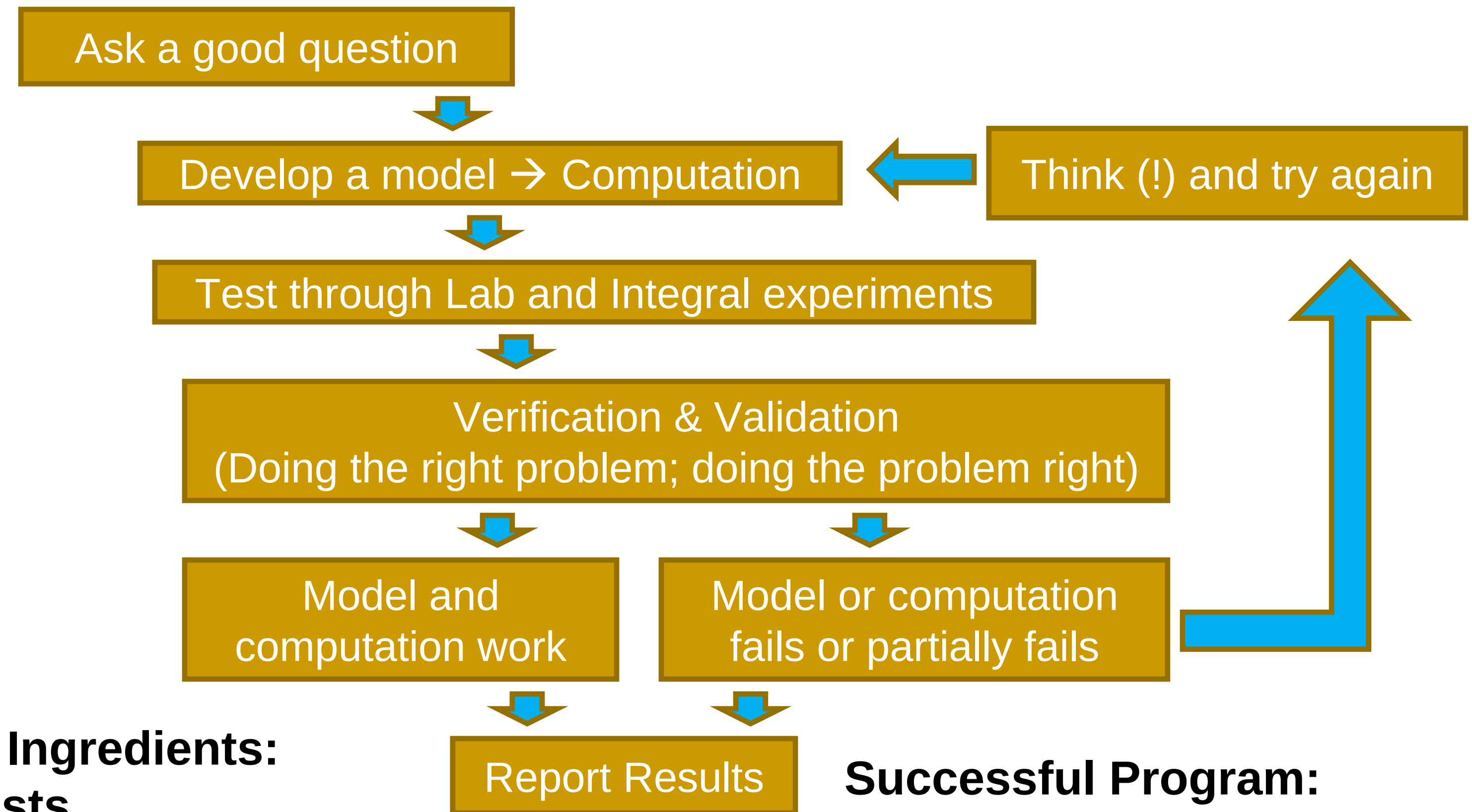
U.S. DEPARTMENT OF ENERGY

Science, tools, and algorithms



U.S. DEPARTMENT OF ENERGY

Computation as a tool in science



Required Ingredients:

1) Theorists
2) Computational Scientists
3) Experimentalists
4) Applied Mathematicians
5) Computer Scientists

Successful Program:

1) Guides experiments
2) Quantifies uncertainties
3) Yields solutions/insights
4) Eliminates tunable parameters

U.S. DEPARTMENT OF ENERGY

Tools have changed rapidly: power

These were our supercomputers in the 1970’s and 1980’s

1986:
X-MP/48 ~220 Mflop sustained
120-150kW (depending on model)
$40M for computer+disks (FY09$)

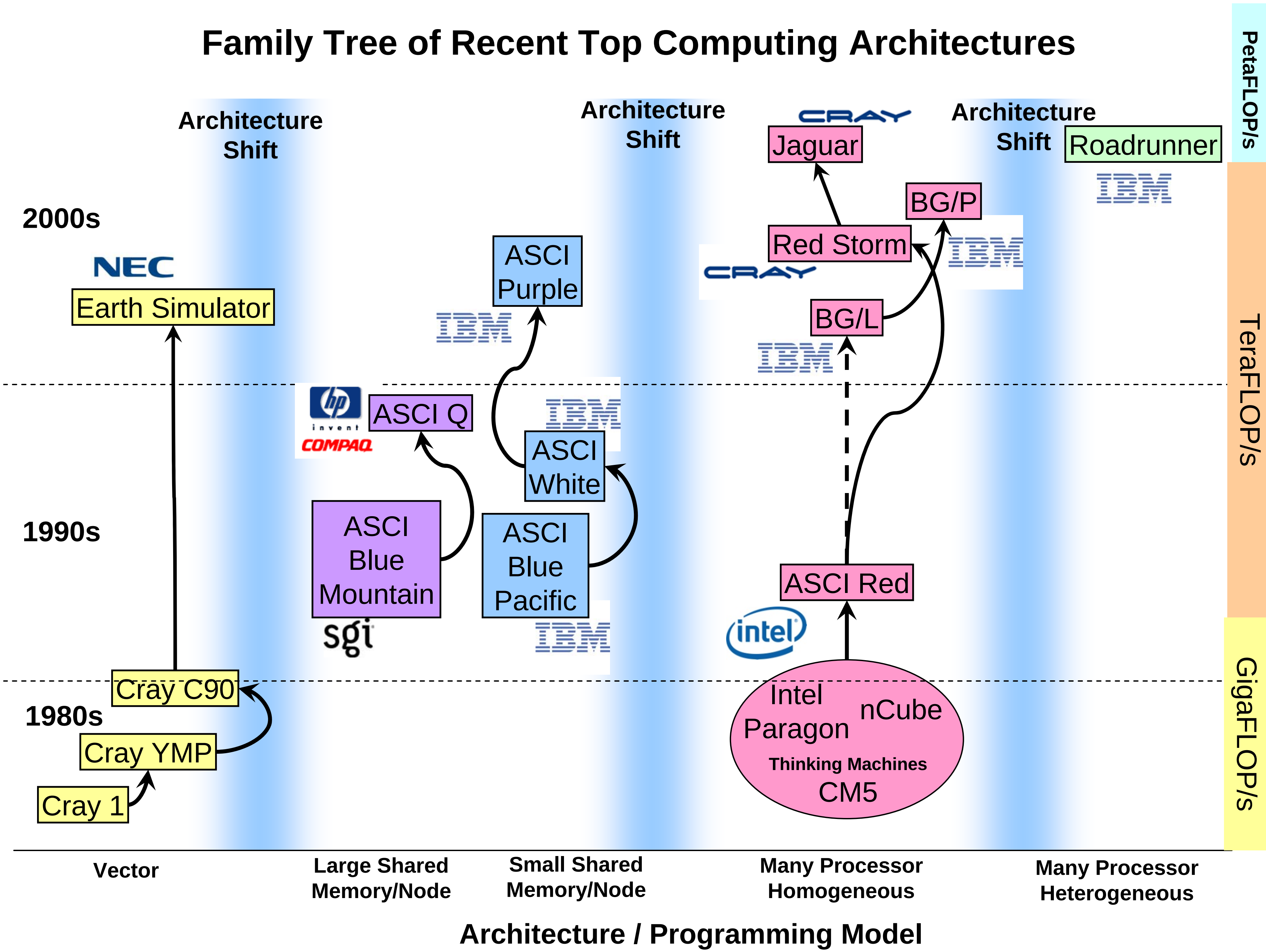
Today:

NNSA:
Roadrunner at 1.105 PF (LINPACK)
LANL; 2.5 MW

SC/ASCR:
Jaguar at 1.059 PF (LINPACK)
ORNL; 6.9 MW

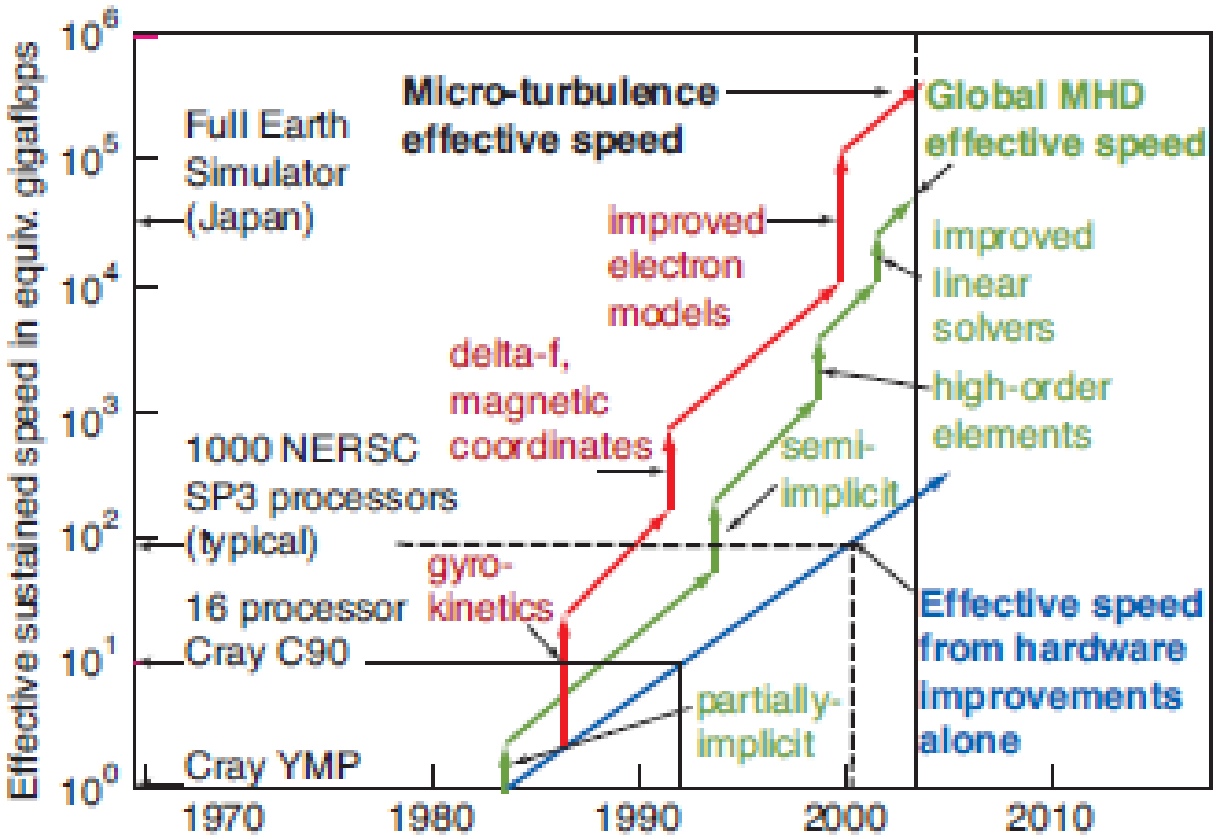
Factor $5x10^6$ in speed
Factor of 18 in power

U.S. DEPARTMENT OF ENERGY



Family Tree of Recent Top Computing Architectures
Architecture Shift
Architecture Shift
Architecture Shift
PetaFLOP/s
TeraFLOP/s
GigaFLOP/s
2000s
1990s
1980s
NEC
Earth Simulator
Cray C90
Cray YMP
Cray 1
ASCI Q
COMPAQ
ASCI Blue Mountain
sgi
ASCI Purple
IBM
ASCI White
ASCI Blue Pacific
CRAY
Jaguar
Red Storm
BG/P
BG/L
ASCI Red
intel
Intel Paragon
nCube
Thinking Machines
CM5
Roadrunner
Vector
Large Shared Memory/Node
Small Shared Memory/Node
Many Processor Homogeneous
Many Processor Heterogeneous
Architecture / Programming Model

Algorithms and models also yield solutions



Magnetic fusion energy "effective speed" increases
Source: A Science-Based Case for Large-Scale Simulation (SCaLeS) Volume 2

A balanced R&D portfolio includes all three:
- -- faster hardware
- -- better mathematical models
- -- improved computational algorithms

Exascale challenges going forward

- Scientific justification
  - How will Exascale help to solve important problems?
  - Not all important problems are extreme scale
- Breakthroughs hardware and software
  - Power consumption; memory bandwidth; communications; …
  - New algorithms: such as O(n) methods; usability
- Building interdisciplinary communities
  - Integrate the domain knowledge of theorists, experimentalists (lab and integral), computational and computer scientists, and applied mathematicians
  - Collaborating with NNSA

U.S. DEPARTMENT OF ENERGY

Questions/Comments?