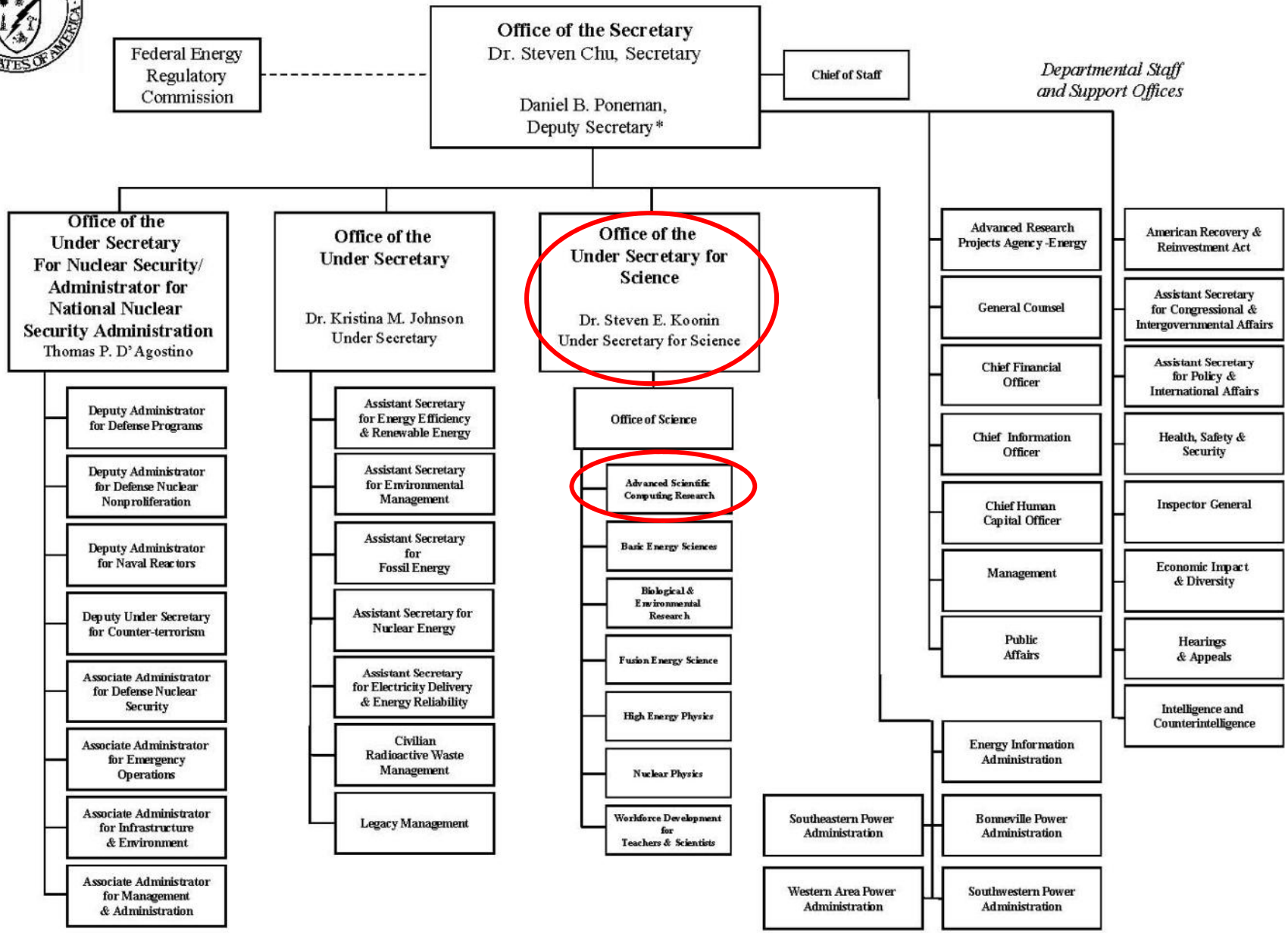
U.S. DEPARTMENT OF ENERGY

Simulations in Science, Energy, and National Security

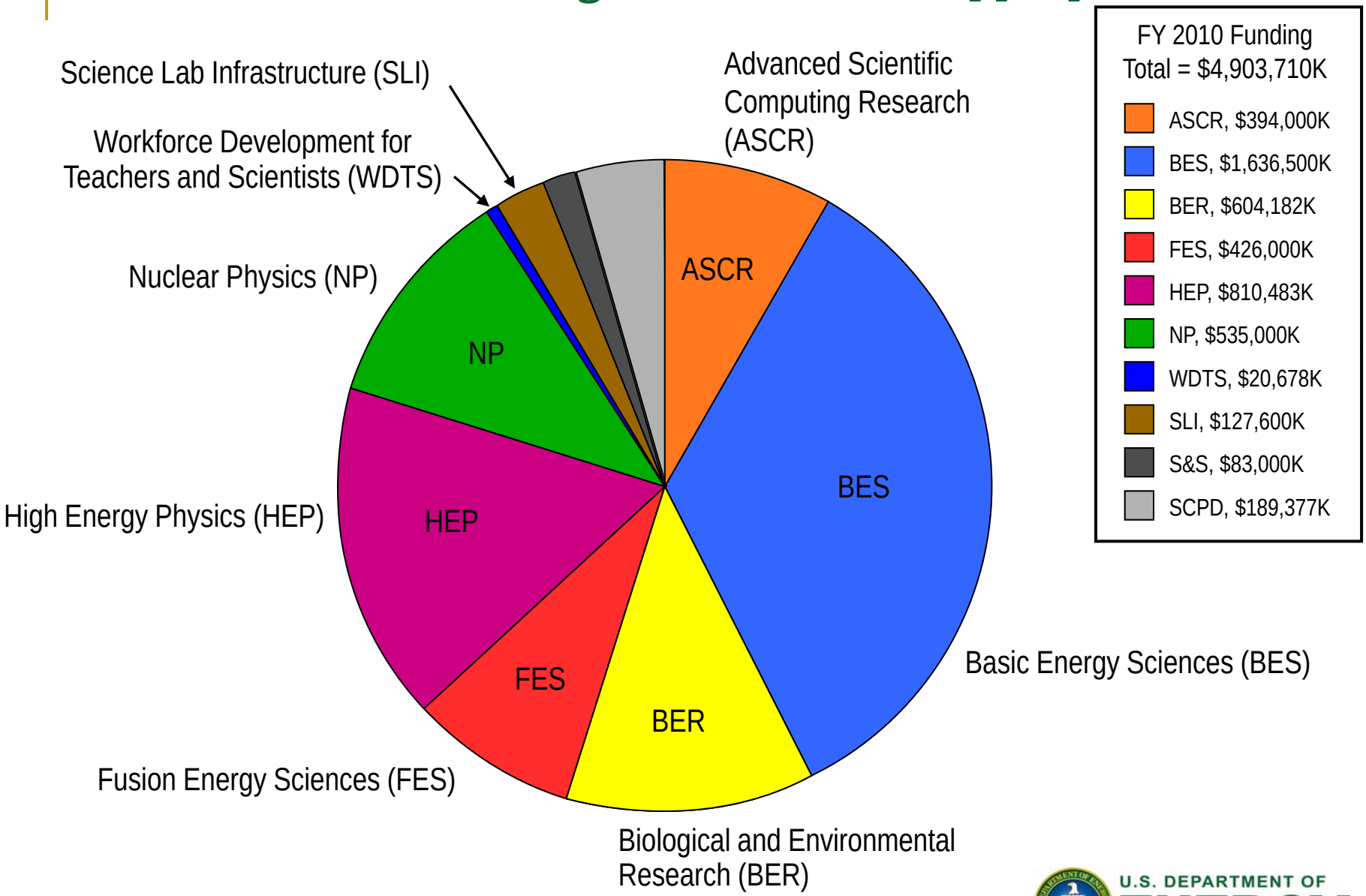
Steven E. Koonin
Under Secretary for Science
US Department of Energy
July 12, 2010
SciDAC

DEPARTMENT OF ENERGY



*The Deputy Secretary also serves as the Chief Operating Officer

Office of Science Programs: FY 2010 Appropriation

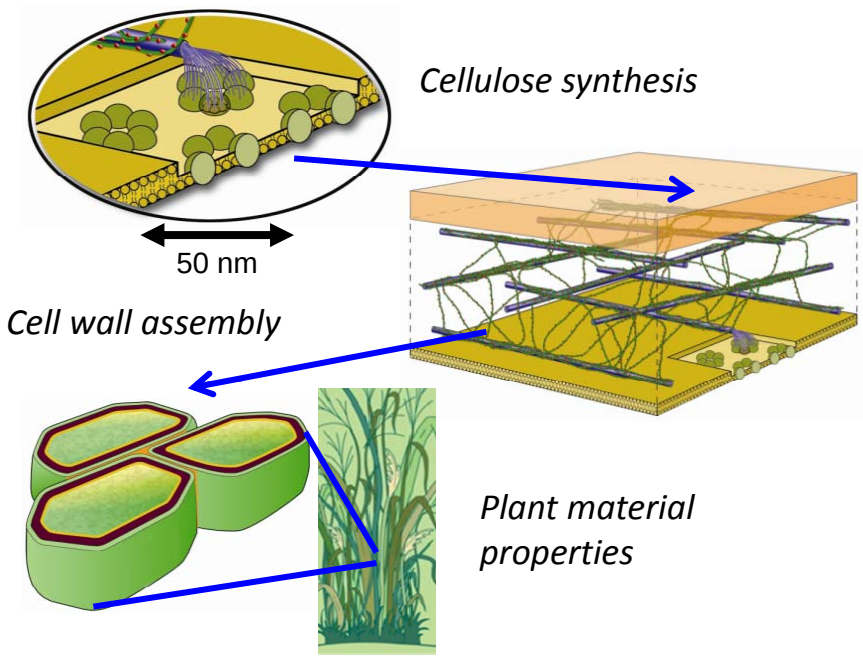


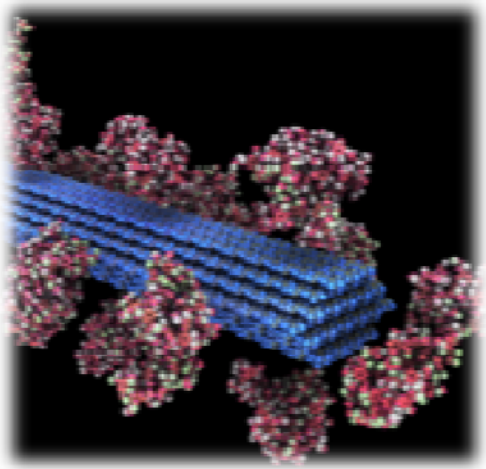
DOE missions

DOE Secretary, Dr. Steven Chu

- Sustain **basic research,** discovery and mission driven
- Catalyze a transformation of the national/global **energy system**
- Enhance **nuclear security**
- Contribute to **US competitiveness** and jobs

Basic Research





- How do we determine US position in various scientific fields?
- How can we balance resources in basic research between fields close to vs distant from applications?
- How do agencies talk to the public, Congress?
- How can we improve climate science?

Accelerating Energy Transformation

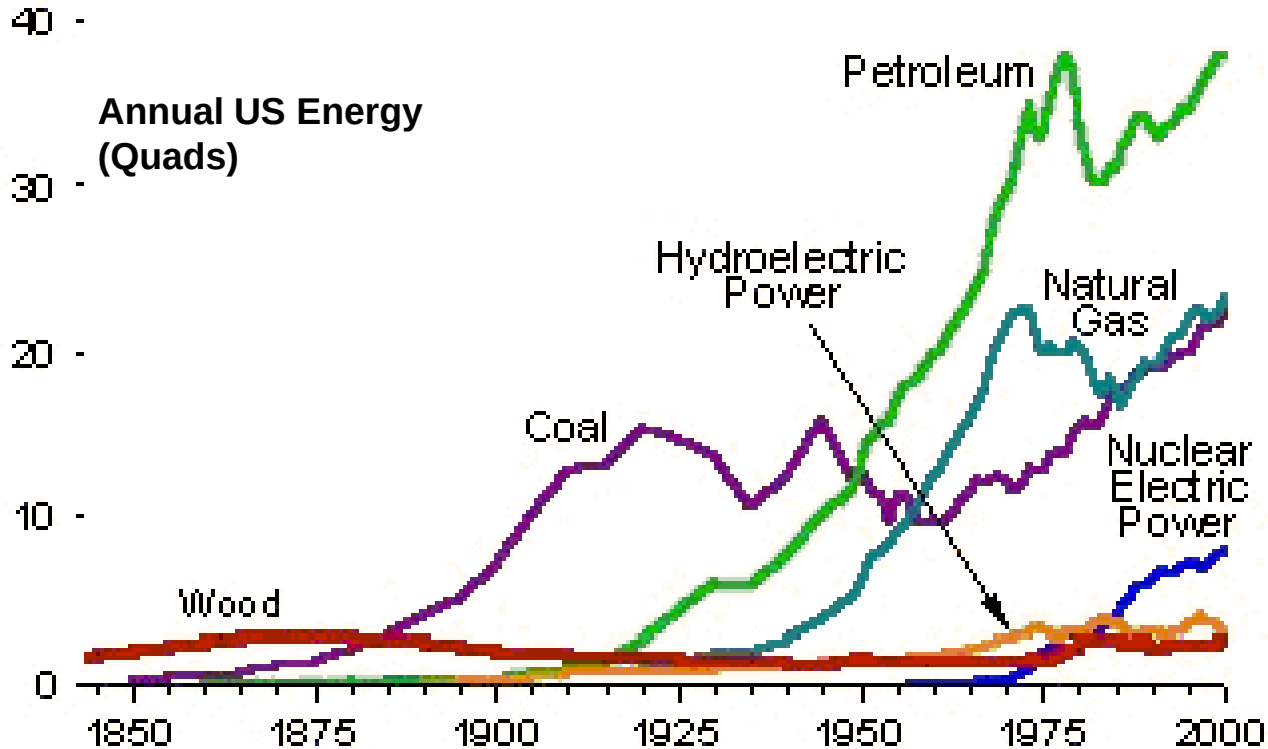
Energy security:

3.5 M bbl/day reduction in crude use

Greenhouse gas emissions:

17% reduction by 2020,

83% by 2050



- Changing the historically decadal timescale?
- S&T engaging society and industry? The best research structures?
- Coupling basic and applied research?
- Formulating/Communicating sensible policy?

U.S. DEPARTMENT OF ENERGY

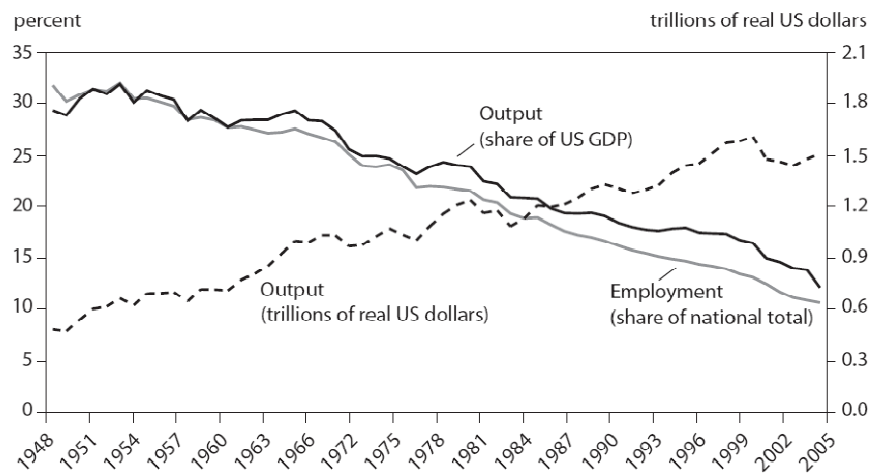
Nuclear Security

- Maintain technical base?
- Keep staff engaged?
- Energy prospects for the National Ignition Facility?
- Exploit simulation capabilities

US Competitiveness

- How do we get to a deep understanding of the issues?
- How do we get public dialog/understanding?
- What is the US strategy?
- How do we execute?
- What role do scientists and S&T play?

Trends in US Manufacturing



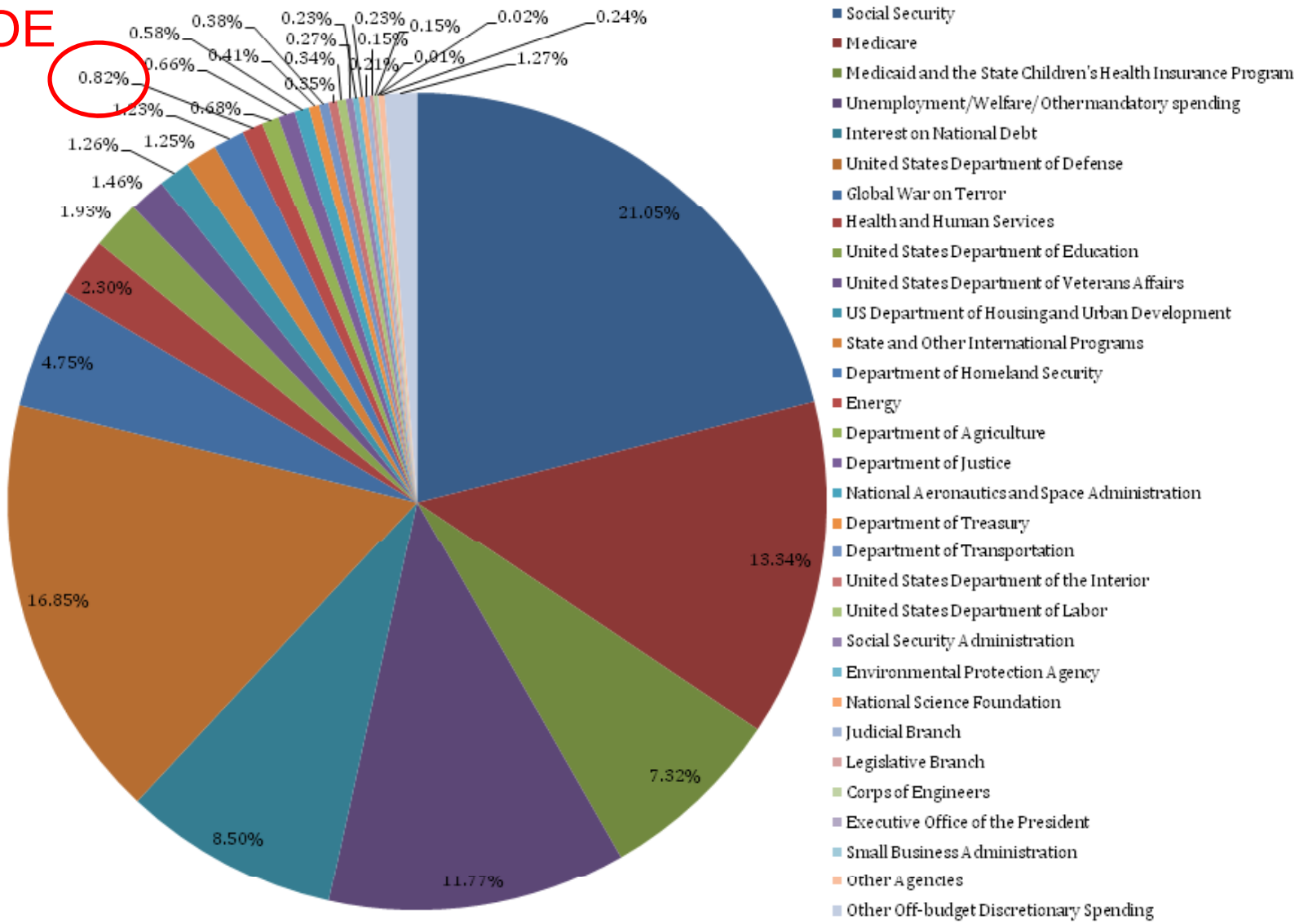
Sources: US Department of Commerce, Bureau of Economic Analysis, Industry Economic Accounts,

"The United States led the world's economies in the 20th century because we led the world in innovation. Today, the competition is keener; the challenge is tougher; and that is why innovation is more important than ever. It is the key to good, new jobs for the 21st century." --*President Barack Obama, August 5, 2009*

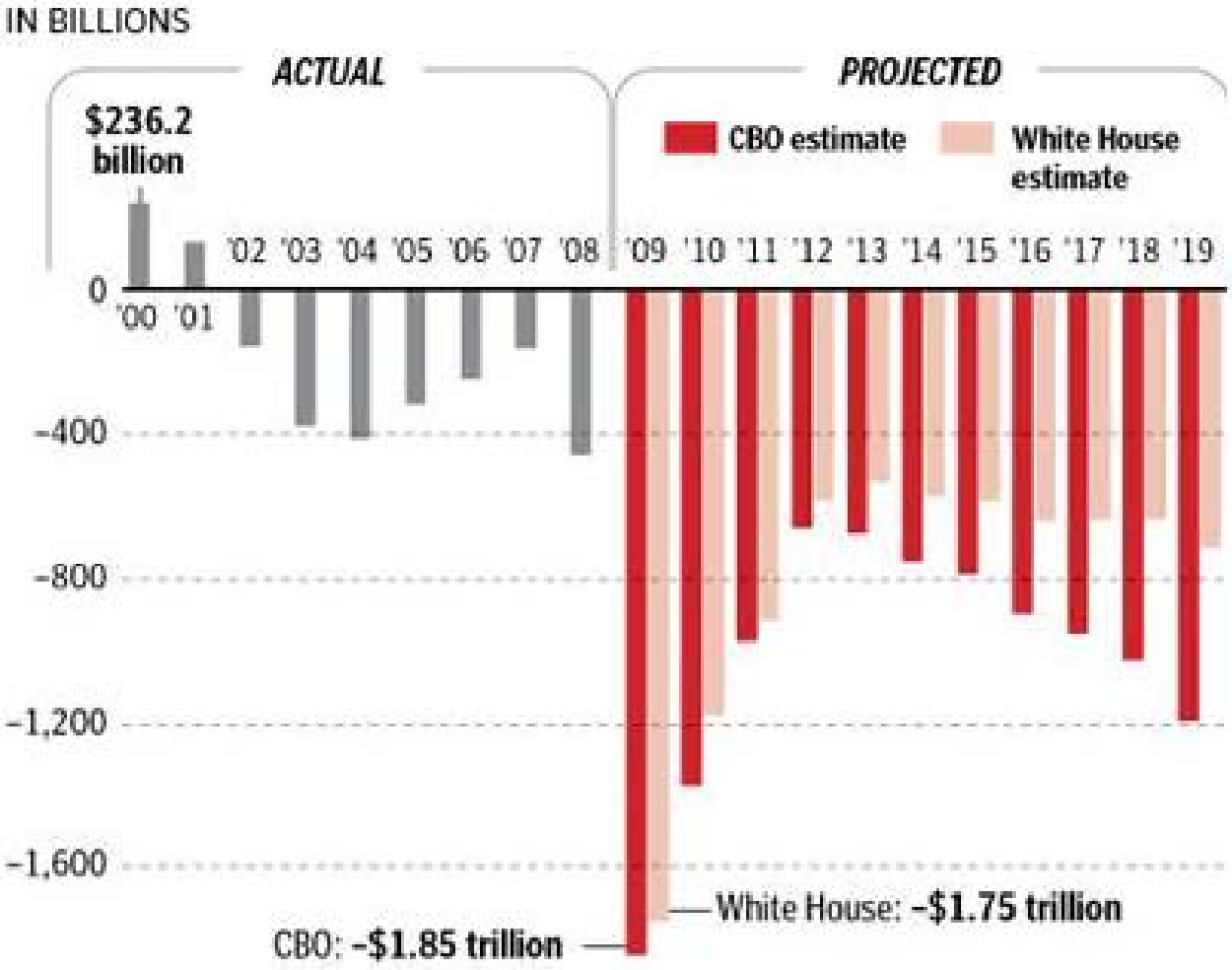
U.S. DEPARTMENT OF ENERGY

FY09 Federal Spending

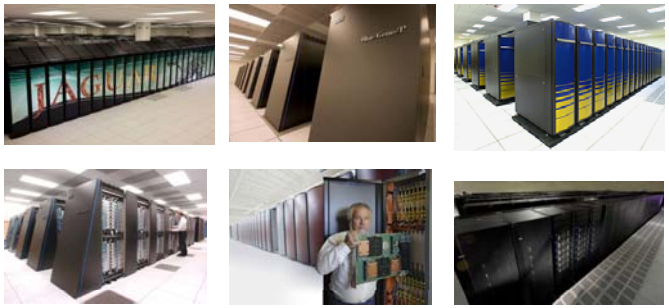
DOE



Federal deficit projections



DOE provides extreme scale computing today: 15 years of world leadership



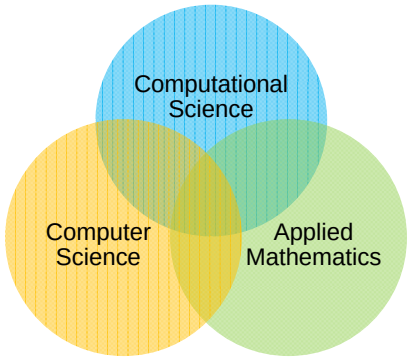
The Office Of Advanced Scientific Computing Research

NNSA
Advanced Simulation and Computing

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	LBNL	0.266 PF	2008 (18)

INCITE: 2.5x oversubscribed

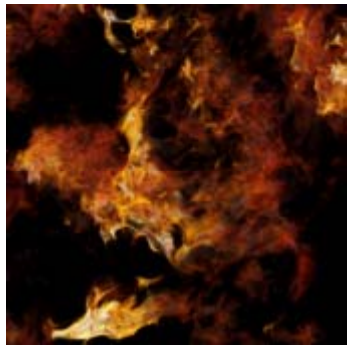


ASC and ASCR *provide much more than machines*:

- Applications (Computational Science)
- Algorithms (Applied Mathematics)
- Systems (Computer Science)
- Integration (SciDAC, Campaigns)

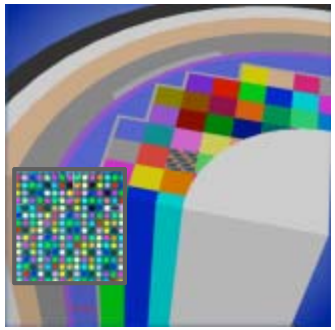
U.S. DEPARTMENT OF ENERGY

Simulations have come of age in Science and National Security



Turbulence

Understanding the statistical geometry of turbulent dispersion of pollutants in the environment.

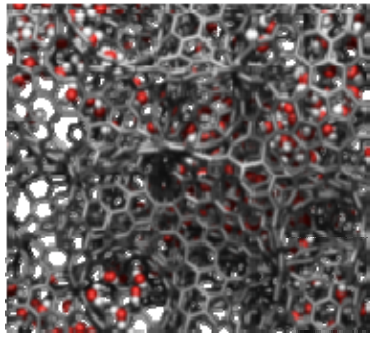


Nuclear Energy

High-fidelity predictive simulation tools for the design of next-generation nuclear reactors to safely increase operating margins.

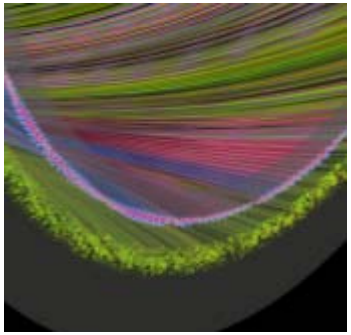
Energy Storage

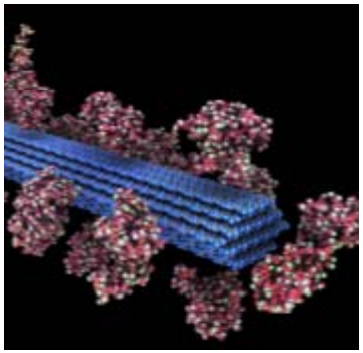
Understanding the storage and flow of energy in next-generation nanostructured carbon tube supercapacitors



Fusion Energy

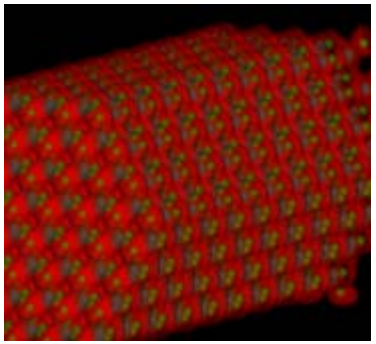
Substantial progress in the understanding of anomalous electron energy loss in the National Spherical Torus Experiment (NSTX).





Biofuels

A comprehensive simulation model of lignocellulosic biomass to understand the bottleneck to sustainable and economical ethanol production.



Nano Science

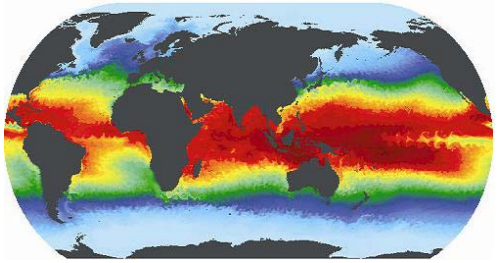
Understanding the atomic and electronic properties of nanostructures in next-generation photovoltaic solar cell materials.

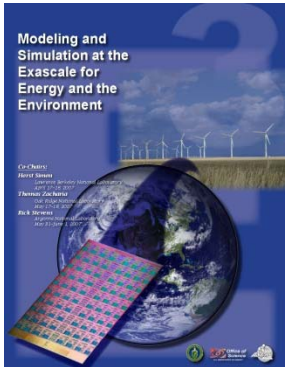
All known sustained petascale science applications to date have been run on OLCF system

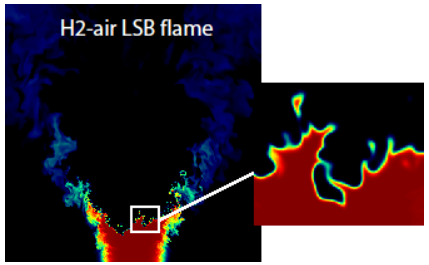
U.S. DEPARTMENT OF ENERGY

Simulation has become an important means toward innovation in science and national security: Extreme Scale Workshops

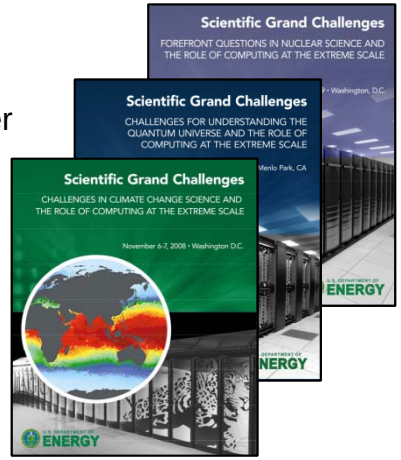
- Town Hall Meetings April-June 2007
- Scientific Grand Challenges Workshops November 2008 – October 2009
  - Climate Science (11/08)
  - High Energy Physics (12/08)
  - Nuclear Physics (1/09),
  - Fusion Energy (3/09),
  - Nuclear Energy (5/09) (with NE)
  - Biology (8/09)
  - Material Science and Chemistry (8/09),
  - National Security (10/09) (with NNSA)
- Cross-cutting workshops
  - Architecture and Technology (12/09)
  - Architecture, Applied Mathematics and Computer Science (2/10)
- Meetings with industry (8/09, 11/09)
- External Panels
  - ASCAC Exascale Charge (FACA)
  - Trivelpiece Panel

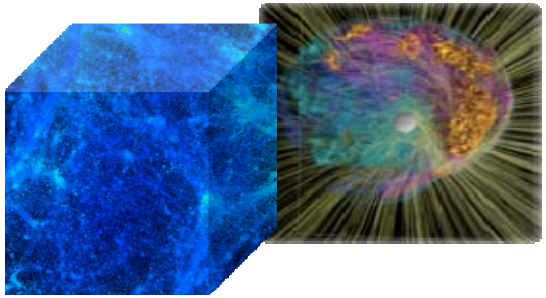






MISSION IMPERATIVES





FUNDAMENTAL SCIENCE

U.S. DEPARTMENT OF ENERGY

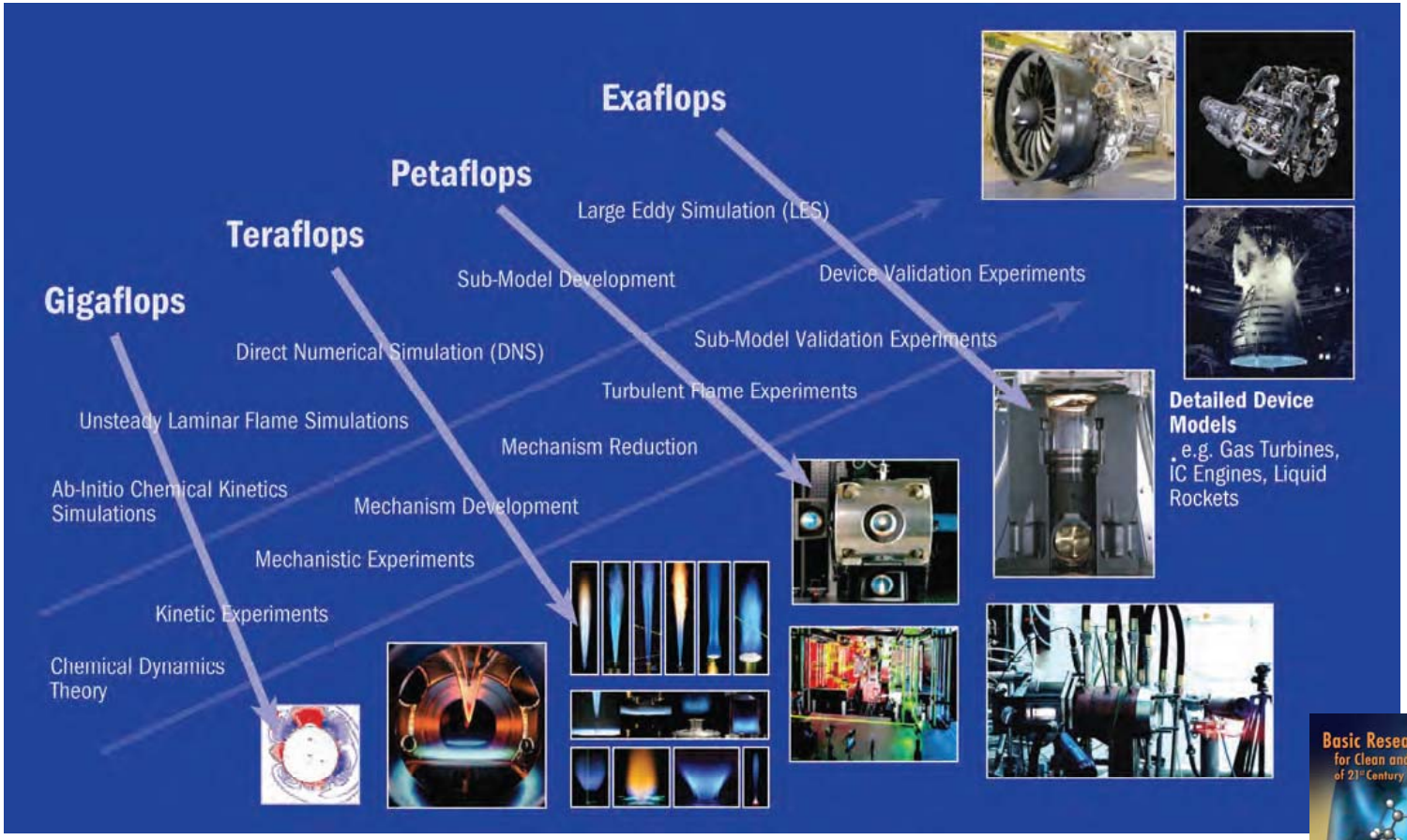
Simulations to accelerate innovation for competitiveness: Two examples

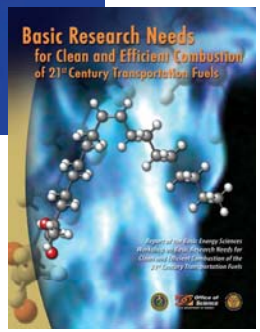
Cummins achieved a milestone in engine design by bringing a diesel engine, the 2007 ISB 6.7 liter, to market solely with computer modeling and analysis tools. The only testing was after-the-fact to confirm performance. Cummins achieved a reduction in development time and cost (estimated to be about 10 to 15% for this first effort). As important, they realized a more robust design, improved mileage, and met all environmental and customer constraints.

Goodyear's Assurance® Triple Tred all-weather tire was its first product designed using predictive modeling simulation tools developed in conjunction with Sandia National Laboratories. This tire and the subsequent products utilizing advanced modeling capabilities resulted in a factor of three reduction in product development time and led to record profits for Goodyear.

U.S. DEPARTMENT OF ENERGY

Combustion simulation initiative in FY11 to accelerate innovation



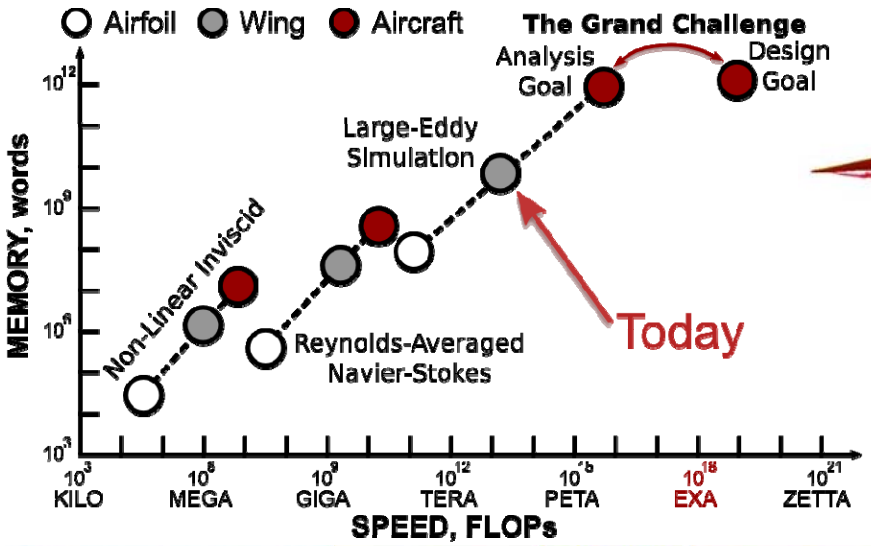


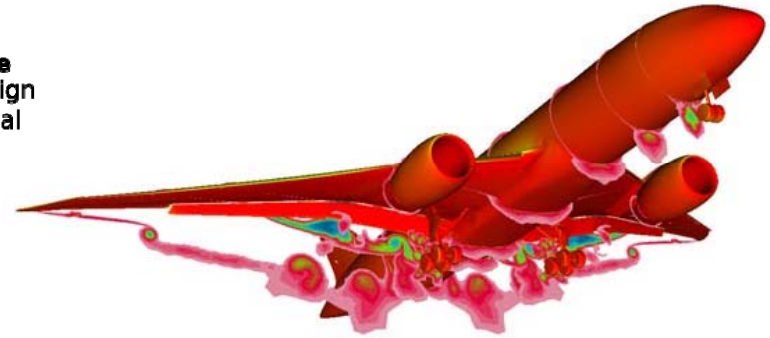
Develop a validated, predictive, multiscale, combustion modeling capability that can optimize the design and operation of evolving fuels in advanced engines and power plants.

Thousands of design iterations – each corresponding to a high-fidelity multiscale simulation –would accelerate optimization and implementation of new technologies.

U.S. DEPARTMENT OF ENERGY

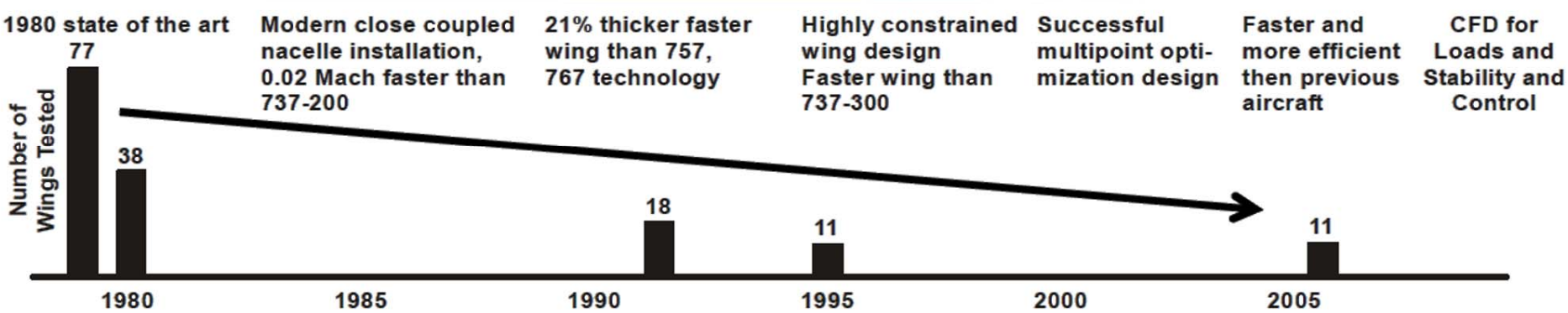
Boeing: Innovation for flight





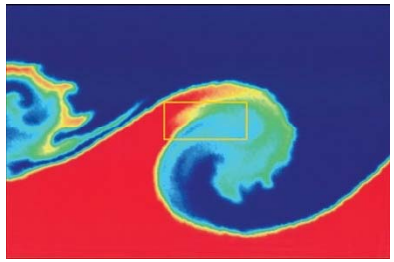
"High Performance Computing has Fundamentally Changed the Way that Boeing Designs Flight Vehicles."

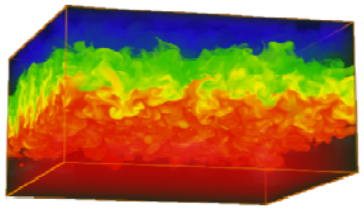
-Director, Boeing Commercial Airplanes



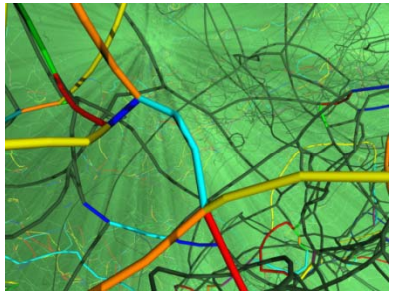
Predictive simulations for nuclear security

- New materials for safety and surety
- Performance of aging systems
- Advanced surety features
- Uncertainty Quantification (UQ)





Atomic level processes initiating macroscopic hydrodynamic instabilities



Fundamental processes driving material performance and aging

Advanced surety features

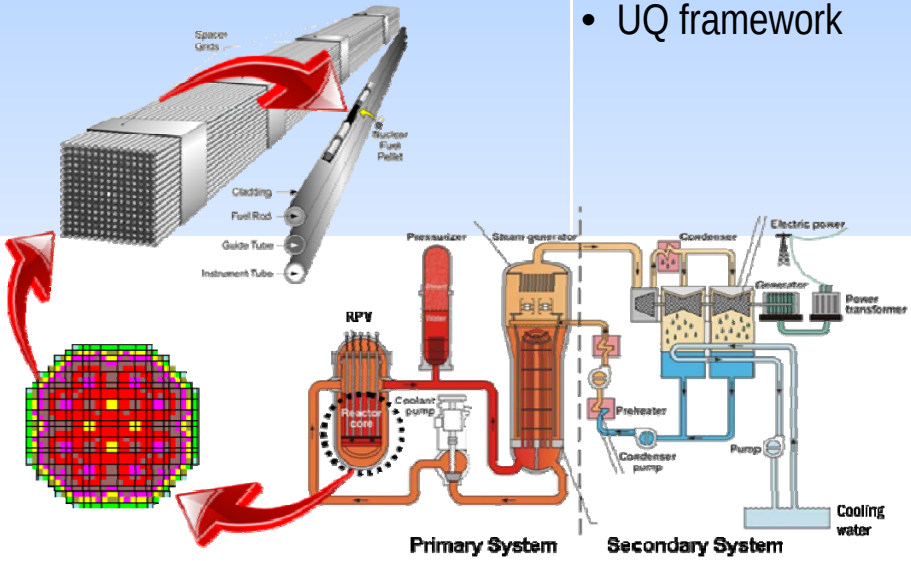
Rapid assessment of proliferant devices

- Stockpile stewardship will remain challenging in the future.
- Predictive simulations are essential to maintaining a safe, secure, and *smaller* stockpile
- Exascale computing would more fully resolve future stockpile concerns

U.S. DEPARTMENT OF ENERGY

CASL vision: Create a virtual reactor for *predictive* simulation of LWRs

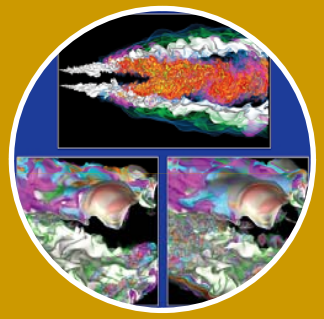
Leverage	Develop	Deliver
• Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications • Existing systems and safety analysis simulation tools	• New requirements-driven physical models • Efficient, tightly-coupled multi-scale/multi-physics algorithms and software with quantifiable accuracy • Improved systems and safety analysis tools • UQ framework	• An unprecedented predictive simulation tool for simulation of physical reactors • Architected for platform portability ranging from desktops to DOE's leadership-class and advanced architecture systems (large user base) • Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors • Base M&S LWR capability



Simulations for Innovation

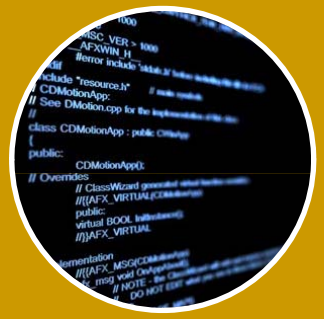
Training a computationally aware workforce

- Education
- Workforce Training
- Simulations Extension Service



Industry Partnerships

- Combustion
- The electric grid
- Nuclear energy
- CCS
- Materials



Software development and validation

- Work with Industry to develop scalable codes for applications

Midrange expertise

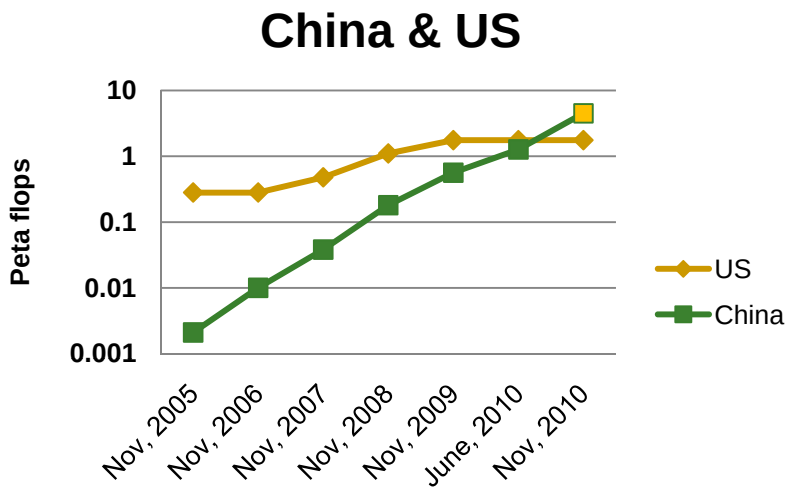
- Provide Industry cycles and infrastructure support to port their codes

Simulation Innovation Elements

Enhance economic competitiveness by making application of simulations a differentiating capability for U.S. industry

U.S. DEPARTMENT OF ENERGY

Exascale: Competitiveness

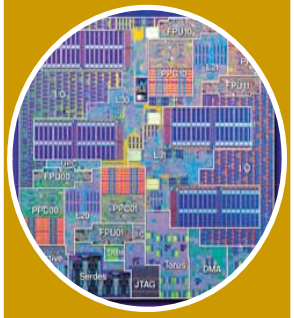


- US leads today in HPC
- China is pursuing HPC vigorously;
- By November, 2010:
  - 3-6 PF machine Chinese integrated from US accelerators by November
  - 1 PF full Chinese machine
  - China likely #1 on the Top 500 list in November
- HPC "feeds itself"

• US Companies involved in HPC

U.S. DEPARTMENT OF ENERGY

Exascale Program Elements



Platform R&D

2 Vendor Tracks

- Power
- Integration
- Risk Mitigation

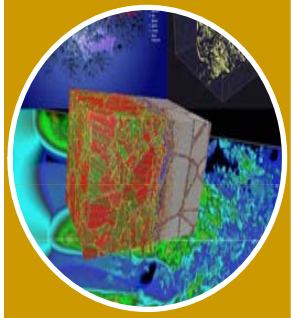
Critical Technologies

(everyone benefits)

- Memory
- Nonvolatile storage
- Optics

Software and Environments

- Operating environment
- Systems Software
- System reliability
- Programming model



Co-design

- Performance models
- Simulators
- Applications integration with vendors

Platforms

- Early prototypes to ensure component integration and usefulness
- Risk mitigation for vendors – Non recoverable engineering cost

Exascale Elements

Today's capability platform becomes tomorrow's desktop

U.S. DEPARTMENT OF ENERGY

What can a scientist do?

- Help advocate for basic research
  - Your field and others
  - Applications can help make the case
- Work with DOE to
  - Bring simulation to industrial innovation
  - Define/develop exascale capabilities
- Understand the bigger problems
  - They *will* affect you, both as a citizen and a scientist
  - Advocate for sensible policies
  - Become involved technically

Questions/Comments?