U.S. DEPARTMENT OF ENERGY | Office of Science

SciDAC Update

July 12, 2010

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Associate Director, Advanced Scientific Computing Research

ASCR Vision

First in Computational Science

Recognized as "Best in Class" advancing science and technology through modeling and simulation

- **Excellence in applied mathematics and computer science research**
  - Research Programs started in 1950's
- **Cross-disciplinary partnerships**
  - In 2000, initiated Scientific Discovery through Advanced Computing
- **Forefront Computing for Science Applications**
  - Top Computing Facilities in the World for Open Science

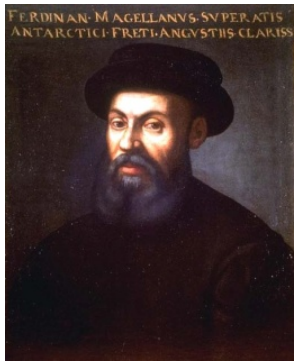
American Recovery and Reinvestment Act

ASCR's Recovery Act Projects ($154.9M)

- **Advanced Networking Initiative ($66.8M)**
  - Testbed to demonstrate and build tools for 100Gbps optical networking technologies
- **Leadership Computing Facility Upgrades ($19.9M)**
  - Six-core upgrade to Oak Ridge LCF machine delivered 2.2 Petaflops
- **Advanced Computer Architectures ($5.2M)**
  - Research on next generation technologies
- **Magellan ($33M)**
  - Research to demonstrate and build tools to enable scientists to utilize cloud computing resources for mid-range computing needs
- **SciDAC-e ($30M)**
  - Supplement and leverage existing SciDAC investments to advance the high performance computational capabilities of the BES - Energy Frontier Research Centers; Extra user support for Energy related projects at the Leadership Computing and NERSC facilities; Applied mathematics research in support of DOE electricity grid efforts.

DOE Explores Cloud Computing

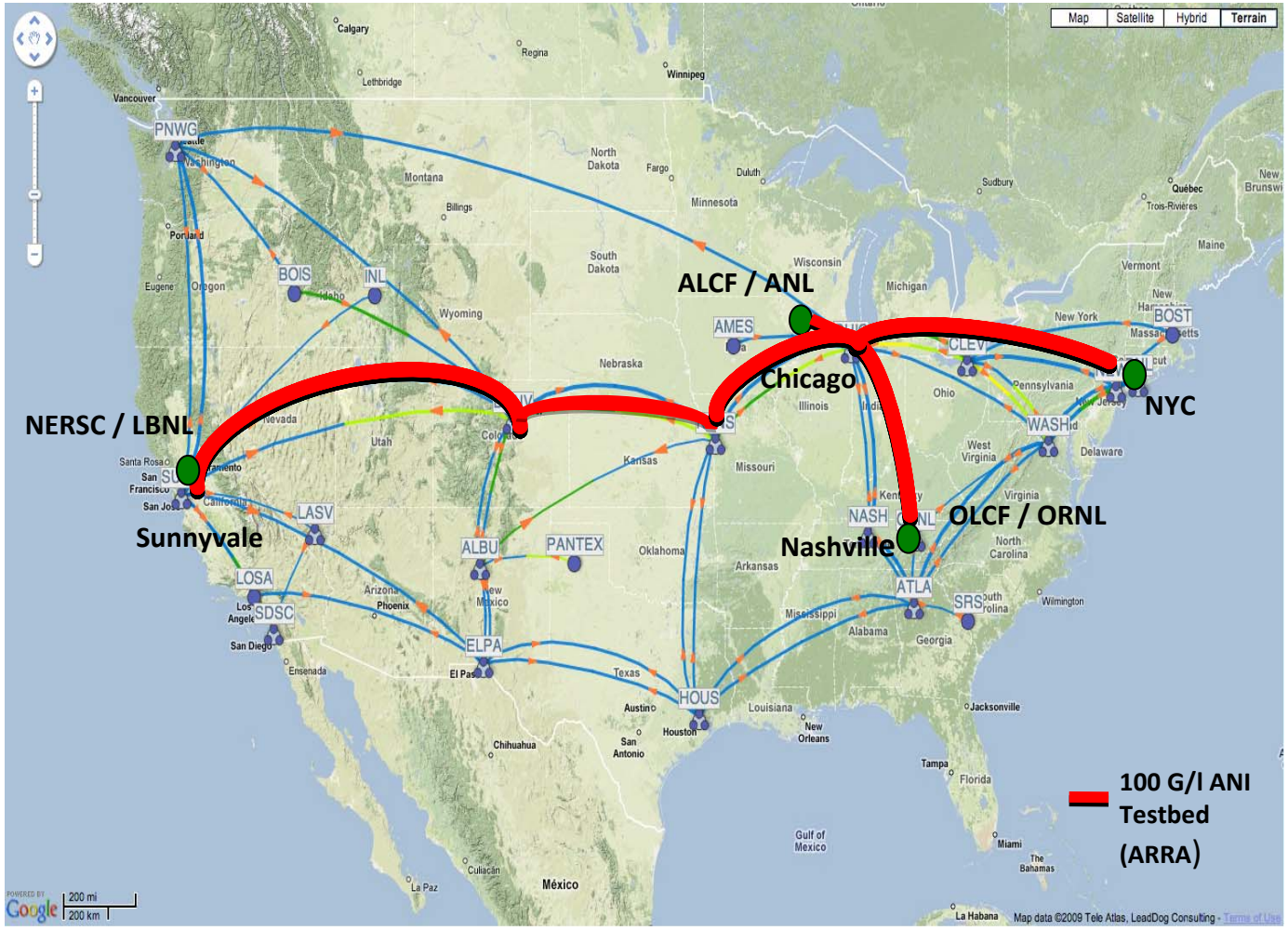
- **The ASCR Magellan Cloud for Science**
  - NERSC and ALCF
  - 100 TF/s across sites
  - Petabyte-scale storage



Open questions:

- Can a cloud serve DOE's mid-range computing needs?
- What hardware and software are needed for a "Science Cloud"?
- How is this unique?

Advanced Networking Initiative



- Prototype 100Gps cards for testing
- Network Test bed is soliciting research projects

SciDAC-e

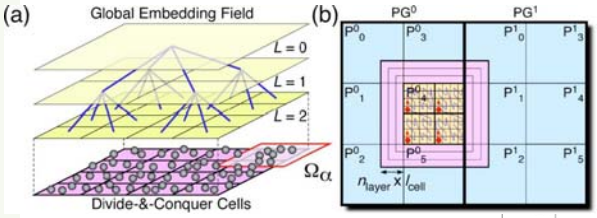
Complex mathematics for smart grids

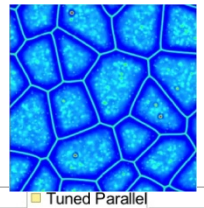
- **Applied mathematics research in support of DOE electricity grid efforts.**
  - *Robust Optimization for Connectivity and Flows in Dynamic Complex Networks,* Lead PI: Balasundaram (Oklahoma State)
  - *Reconfiguring Power Systems to Minimize Cascading Failures: Models and Algorithms,* Co-PIs: Bienstock (Columbia), Wright (UW-Madison)
  - *Approaches for Rare-event Simulation and Decision Making*, Lead PI: Shortle (GMU)
  - *Analysis and Reduction of Complex Networks under Uncertainty*, Marzouk (MIT), Knio (JHU), Ghanem (USC), Najm (SNL)
  - *Optimization and Control of the Electric Power Systems,* Co-PIs: Meza (LBNL), Thomas (Cornell), Lesieutre (UW-Madison)
  - *Advanced Kalman Filter for Real-Time Responsiveness in Complex Systems,* Co-PIs: Huang (PNNL), Welch (UNC-Chapel Hill)
  - *Extending the Realm of Optimization for Complex Systems: Uncertainty, Competition and Dynamics,* Lead PI: Shanbhag (UIUC)
- **All awards made and work has begun.**
- **Plan to conduct programmatic and expert review of progress and results.**

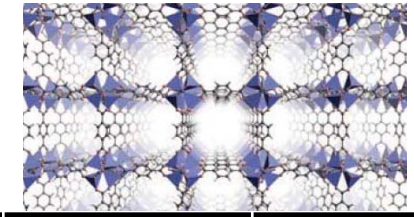
SciDAC-e

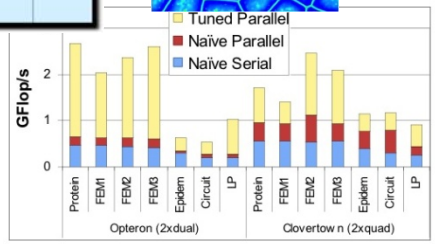
Energy Frontier Research Centers Collaborations

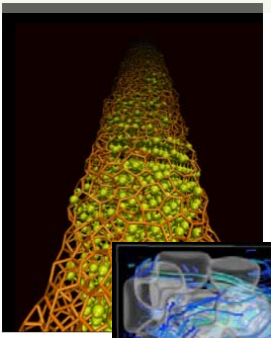
- Supplemental awards to SciDAC CETs & Institutes to support BES EFRCs to develop a high-performance computing capability relevant to the goals of the EFRC
  - 14 awards made with Recovery Act funds in 2010 to APDEC, VACET, IUSV, TOPS, ITAPS, PERI, SDM

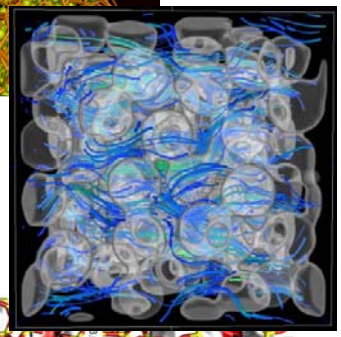


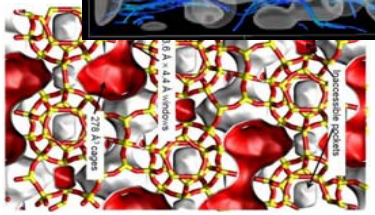










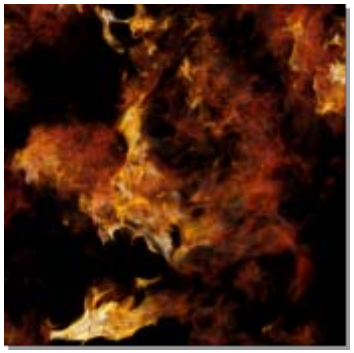


EFRC Category	# Unique EFRCs	# EFRC Collaborations	Award ($K)
Materials Under Extreme Conditions	2	3	1,095
Geological Flows & Carbon Storage	3	6	3,931
Solar & Photovoltaics	5	5	3,379
Material Design	1	2	951
Others	4	4	1,540
TOTAL	15	20	10,895

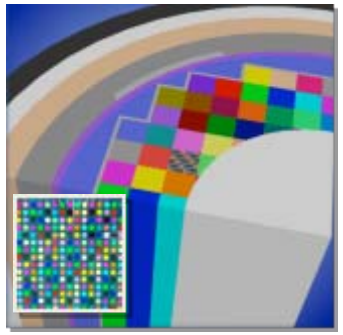
Leadership Computing Upgrade

- Upgrade activities result in less than 10% unscheduled downtime for current users. (2009)
- OLCF Completed acceptance test for quad-core to six-core upgrade of Cray XT5 at Oak Ridge (Q1).
- November, 2009 and June 2010, Jaguar "**World's Most Powerful Computer"** according to TOP500 list

Scientific Progress
Resulting from OLCF Upgrade

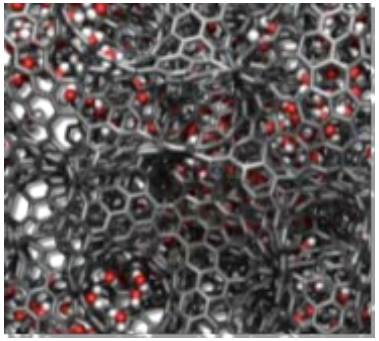


Turbulence
Understanding the statistical geometry of turbulent dispersion of pollutants in the environment.

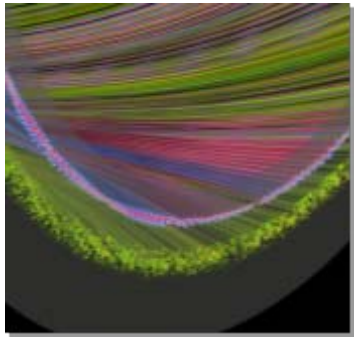


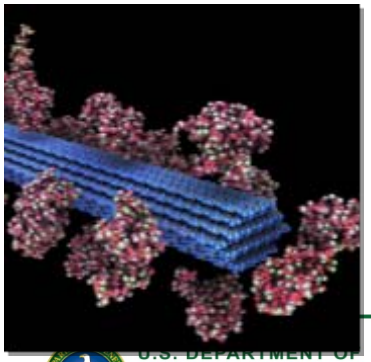
Nuclear Energy
High-fidelity predictive simulation tools for the design of next-generation nuclear reactors to safely increase operating margins.

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

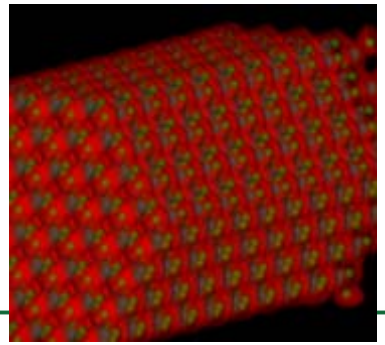


Fusion Energy
Substantial progress in the understanding of anomalous electron energy loss in the National Spherical Torus Experiment (NSTX).





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.

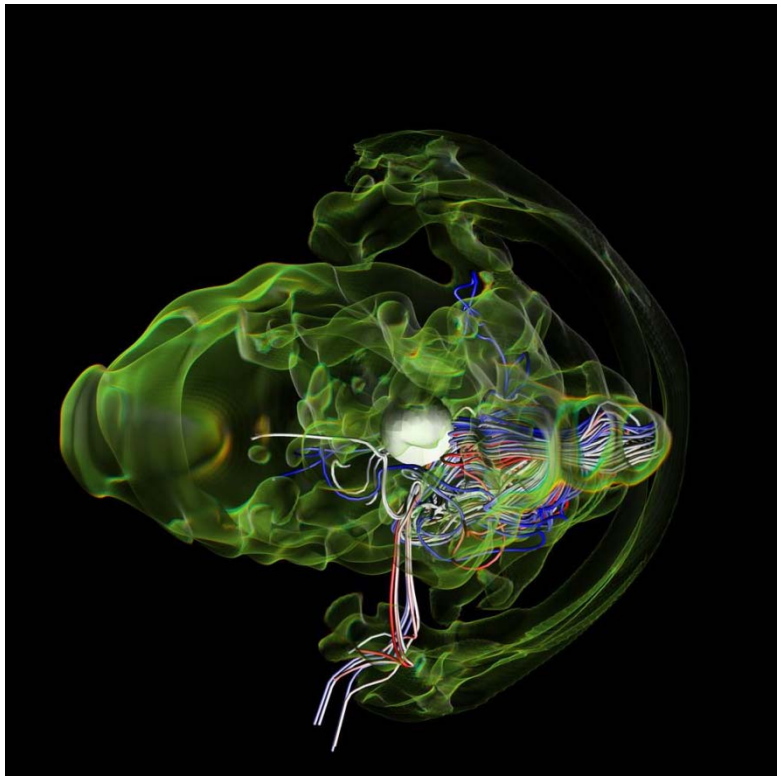
Petascale Science Applications

Science Area	Code	Contact	Cores	Total Performance	Notes
Materials	DCA++	Schulthess	213,120	1.9 PF*	2008 Gordon Bell Winner
Materials	WL-LSMS	Eisenbach	223,232	1.8 PF	2009 Gordon Bell Winner
Chemistry	NWChem	Apra	224,196	1.4 PF	2009 Gordon Bell Finalist
Nano Materials	OMEN	Klimeck	222,720	860 TF	
Seismology	SPECFEM3D	Carrington	149,784	165 TF	2008 Gordon Bell Finalist
Weather	WRF	Michalakes	150,000	50 TF	
Combustion	S3D	Chen	144,000	83 TF	
Fusion	GTC	PPPL	102,000	20 billion Particles / sec	
Materials	LS3DF	Lin-Wang Wang	147,456	442 TF	2008 Gordon Bell Winner
Chemistry	MADNESS	Harrison	140,000	550+ TF	

The role of magnetic fields in the birth of pulsars

Science Results

- **Stationary accretion shock instability(SASI) , a computational *discovery* from earlier INCITE work, is a potential source of spin for pulsars**
- **However, pulsars also have strong magnetic fields that power their synchrotron emission, making them cosmic lighthouses**
- **Large (~100,000 processors) MHD simulations performed with GenASiS show that rapid field amplification does occur, driven by the turbulence caused by the SASI**
- **Confirmed that the general dynamic features of the SASI remained unchanged by magnetic fields**

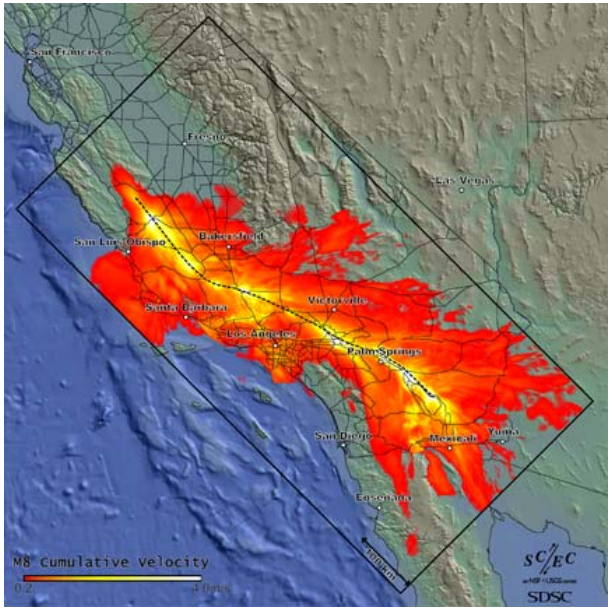


Magnetic field streamlines from a MHD simulation of the stationary accretion shock instability in core-collapse supernovae

Deterministic Simulations of Large Regional Earthquakes

Science Results

- **Configured and ran a 2Hz deterministic wave propagation simulation whose size and resolution (223K cores, 24 hours) represents a breakthrough in computational scalability for seismic hazard research. The simulation provides researchers with high-resolution ground motion time histories all across southern California for this scenario earthquake.**
- **The simulation capability will now be applied to a broader seismic hazard research program that must investigate the sources of uncertainties in simulation ground motion results including alterative rupture models and alternative earth structure models.**
- **This earthquake ground motion simulation will be useful to:**
  - (a) Emergency management agencies evaluating "worst case" earthquake scenarios for California,
  - (b) Building engineers evaluating tall building response to possible future earthquakes,
  - (c) Seismic network operators evaluating whether their current station distribution provides adequate monitoring for large earthquakes, and
  - (d) Seismic hazard modeling groups evaluating how 3D ground motion simulations capture ground motions caused by earthquake directivity and basin amplifications

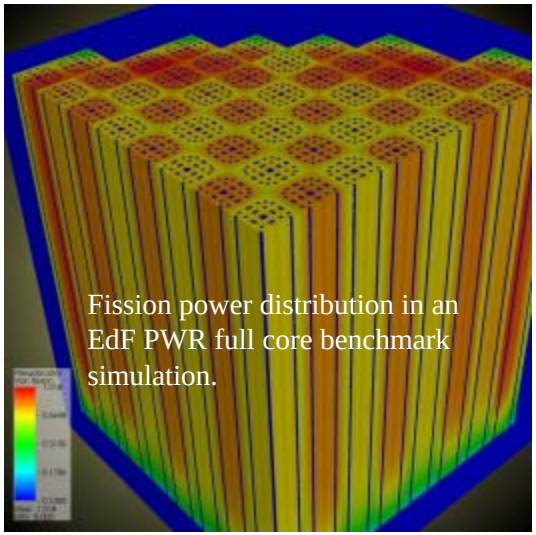


Cumulative ground velocity from a simulated magnitude 8.0 event

Deterministic neutron transport for nuclear energy

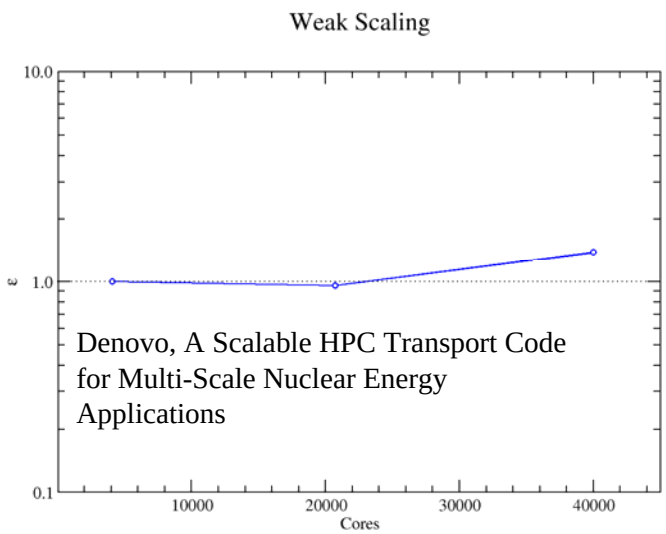
Science Objectives and Impact

- **Strategy:** Perform high-fidelity radiation transport calculations that can be used in a variety of nuclear energy and technology applications, including extensions to multi-physics simulations.
- **Driver:** Next-generation reactor designs require high-fidelity, *ab initio* predictive simulation tools due to a lack of experimental facilities to tune existing, *ad hoc* modeling approaches.
- **Objective:** Use a novel, multi-level parallel decompositions to overcome the wavefront barrier that has limited scaling performance in transport codes.
- **Impact:** High-fidelity transport simulations can reduce the need for expensive experimental facilities, many of which no longer exist. Furthermore, accurate modeling tools can reduce licensing and certification time.



Fission power distribution in an EdF PWR full core benchmark simulation.

Application Performance



Denovo, A Scalable HPC Transport Code for Multi-Scale Nuclear Energy Applications

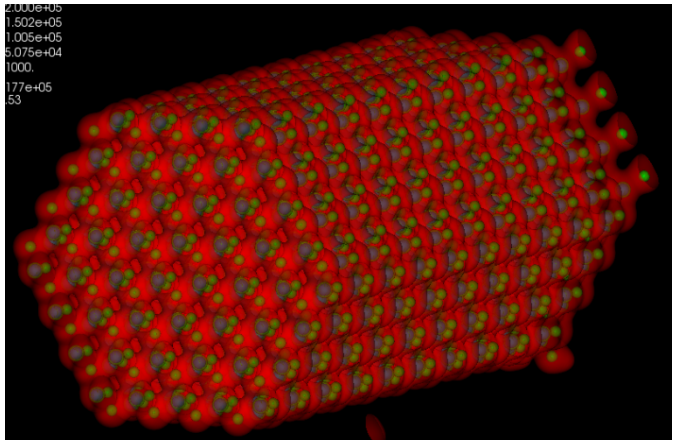
Science Results

- **Largest known simulations of a nuclear reactor**
  - PWR facility: 8.164 Trillion DOF
    - 1.05B cells x 288 directions x 27 groups
  - PWR core: 26 Billion DOF
    - 46M cells x 288 directions x 2 groups
  - BWR assembly: 126 B DOF
    - 528M cells x 120 directions x 2 groups
- **A "game changer": eliminating large sources of uncertainty owing to spatial homogenization**

Large scale electronic structure calculations of nanosystems

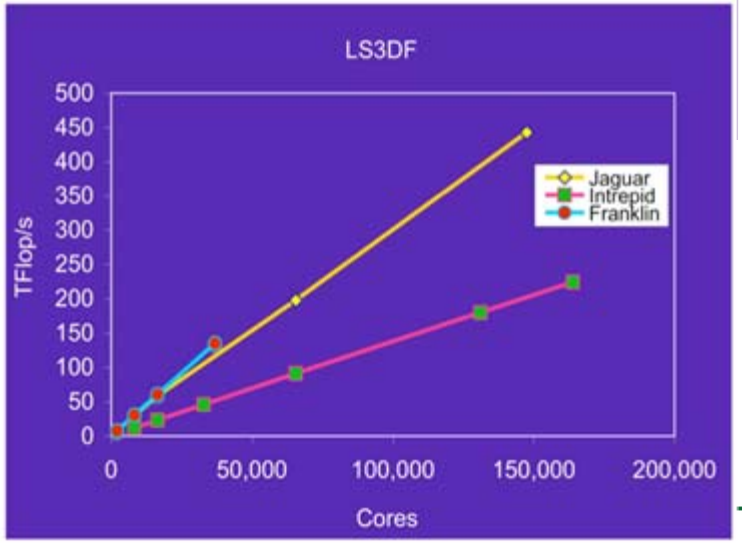
Science Objectives and Impact

- **Strategy: Understand the atomic and electronic structures of surfaces and their coupling to interior eigen states in nanosystems.**
- **Driver: The realistic ZnO surface is relatively simple, with dimerization reconstruction. It provides an ideal case to study the surface electronic structures, and its contribution to the total dipole moment of the system.**
- **Objective: To calculate the ab initio self consistent charge density of a 2010 atom ZnO nanorod with 17520 electrons using LS3DF code.**
- **Impact: The electronic properties of nanosystems are often determined by their surface structures. Understanding the realistic surface electronic structure is one of the biggest challenges in nanoscience**



The total charge density of the ZnO quantum rod

LS3DF Performance



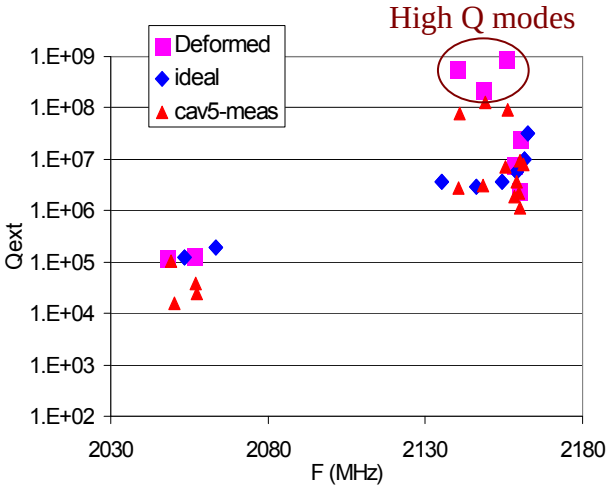
Science Results

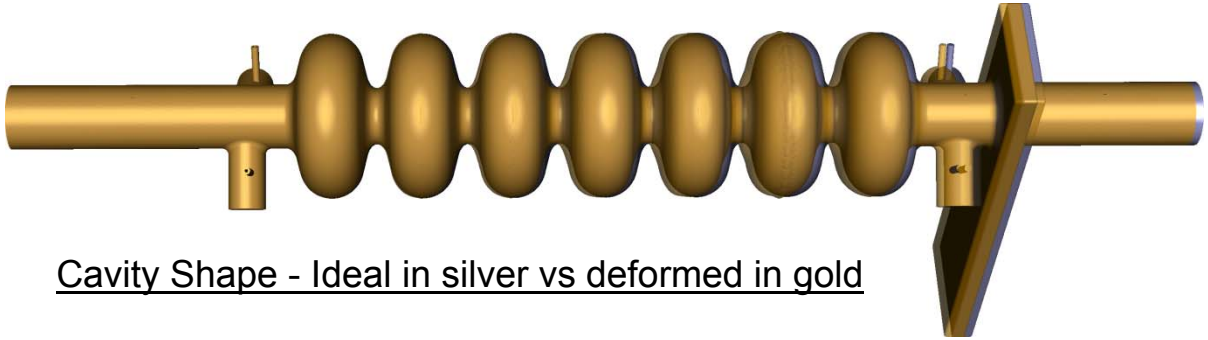
- The first ab initio calculation for II-VI rod with realistic surface structure.
- Found there is a large dipole moment . It has localized electron and hole state at the opposite sides of the rod.
- The surface dimerization has removed the surface states from the interior band gap.

Solving CEBAF BBU Using Shape Uncertainty Quantification

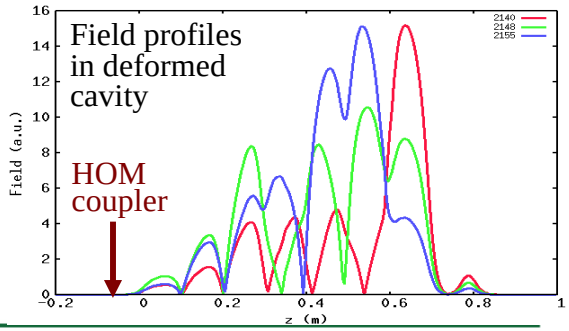
SciDAC Success as a Collaboration between Accelerator Simulation, Computational Science and Experiment – Beam Breakup (BBU) instabilities at well below the designed beam current were observed in the CEBAF12 GeV upgrade of the Jefferson Lab (TJNAF) in which Higher Order Modes (HOM) with exceptionally *high* quality factor (Q) were measured. Using the shape uncertainty quantification tool developed under SciDAC, the problem was found to be a deformation of the cavity shape due to fabrication errors. This discovery was achieved as a team effort between SLAC, TOPS, and JLab which underscores the importance of the SciDAC multidisciplinary approach in tacking challenging applications.

Method of Solution - Using the measured cavity parameters as inputs, the deformed cavity shape was recovered by solving the ***inverse*** problem through an optimization method. The calculations showed that the cavity was 8 mm shorter than designed, which was subsequently confirmed by measurements. The result explains why the troublesome modes have high Qs because in the deformed cavity, the fields shift away from the HOM coupler where they can be damped. This shows that quality control in cavity fabrication can play an important role in accelerator performance. .



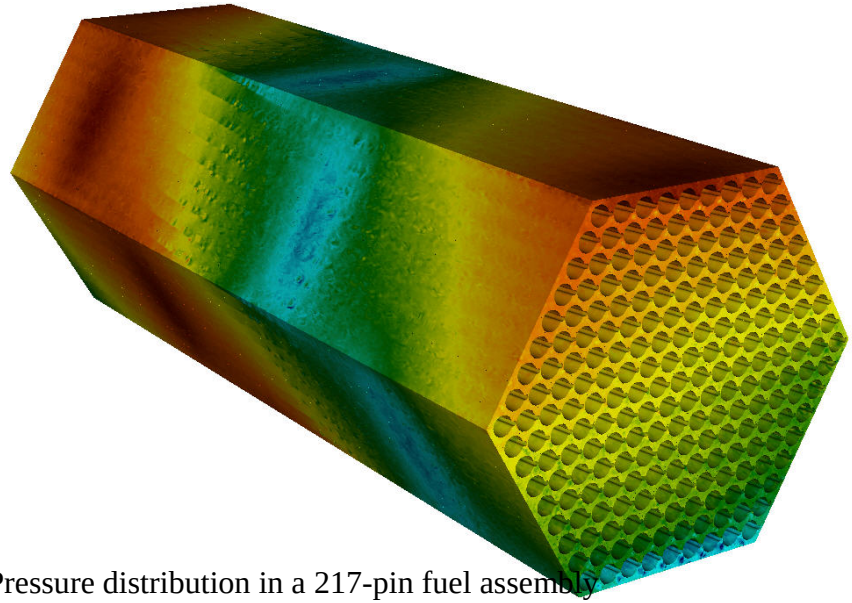


Cavity Shape - Ideal in silver vs deformed in gold



Reactor Core Hydrodynamics

- Large-scale simulations of turbulent thermal transport in sodium-cooled reactor cores are increasing the understanding of fundamental thermal mixing phenomena within advanced recycling reactor (ARR) cores.
  - *Insights gained from these simulations will enable higher power output while increasing safety*
- Potential benefits of ARRs:
  - *Improved safety and economy*
  - *Economical power sources*
  - *Used to recycle spent nuclear fuel*
  - *Reduced loading demands (nearly 100-fold) in geological repositories*
- Work was conducted on the Argonne Leadership Computing Facility BG/P through INCITE awards
  - *Simulation sizes have increased ten-fold in the past 12 months and sustain 80% efficiency on 131,000 cores.*



Pressure distribution in a 217-pin fuel assembly with wire wrap

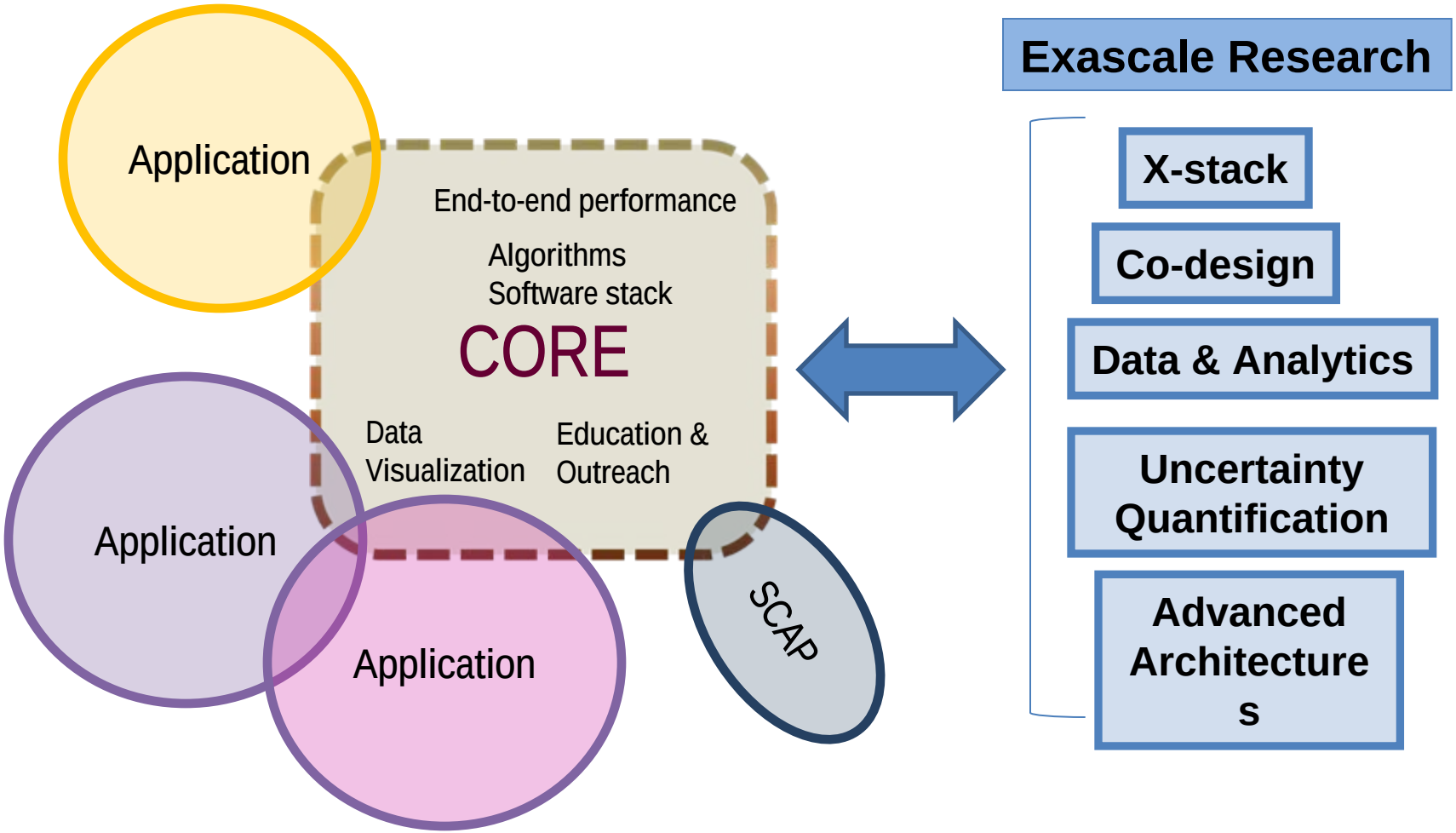
SciDAC Today

SciDAC – Building Community of Computational Scientists

– **Started in 2001; Redesigned and re-competed in 2006**

- **Centers for Enabling Technologies** (CETs) – Research and development in mathematical and computing systems software to support SciDAC application.
- **SciDAC Institutes** are university-led centers of excellence intended to complement CETs with concentrated efforts and a focus on outreach and training.
- **Science Application Partnerships** (SAPs) provide support for multidisciplinary interactions among application domains, computer science and applied mathematicians.
- **The SciDAC Outreach Center** provides a collection point for SciDAC technologies and capabilities intended for industry, academia and other scientific communities.
- **SciDAC Conference** provides an opportunity of computational science community to come together.
- **SciDAC Review** highlights accomplishments of computational science community especially SciDAC and INCITE.

Vision for SciDAC Tomorrow

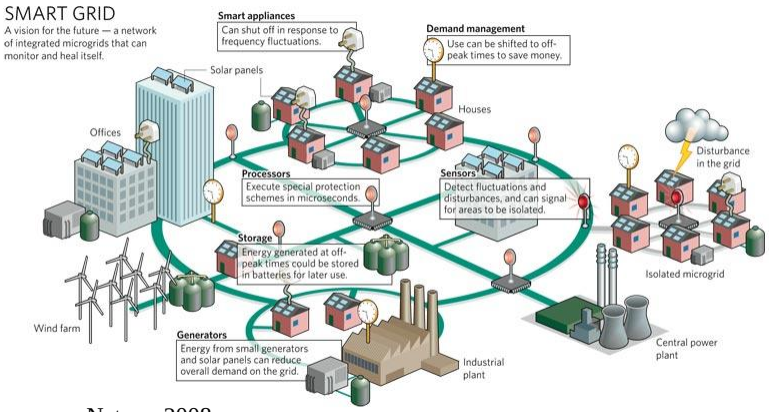


SCAP- Scientific Computation Application Partnership

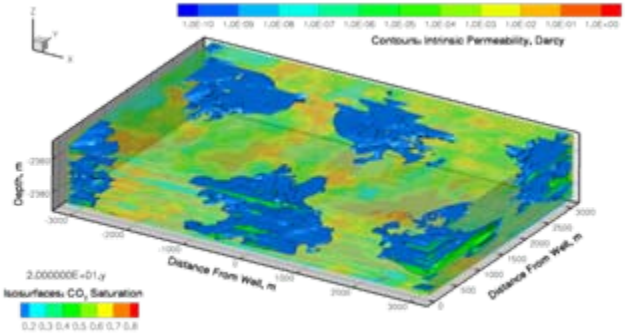
Vision for SciDAC Tomorrow

Computational Applied Science

- **Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production**
  - Reducing time and cost of reactor design and deployment
  - Improving the efficiency of combustion energy systems
  - Safely capturing and sequestering carbon
  - Designing smart buildings and the Electric Power Grid



Nature, 2008



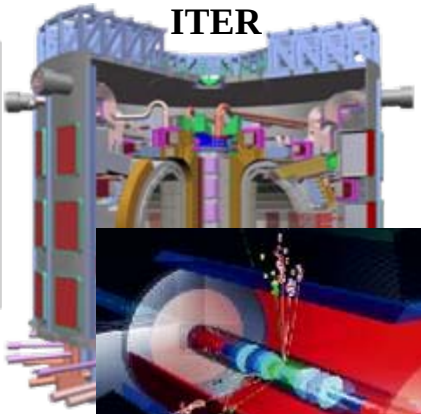
Vision for SciDAC Tomorrow

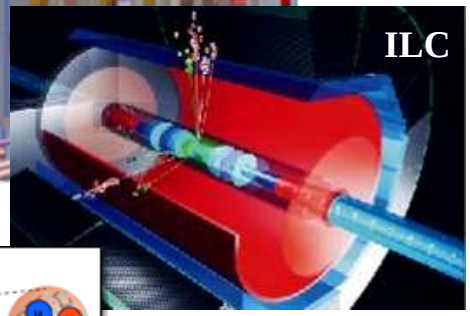
Science at Multi-Petaflops

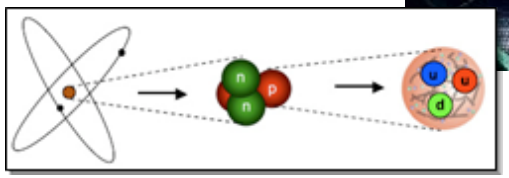
- **High Energy & Nuclear Physics**
  - Dark-energy and dark matter
  - Fundamentals of fission & fusion reactions
- **Facility and experimental design**
  - Effective design of accelerators
  - Probes of dark energy and dark matter
  - ITER shot planning and device control
- **Materials / Chemistry**
  - Predictive multi-scale materials modeling: observation to control
  - Effective, commercial technologies in renewable energy, catalysts, batteries and combustion
- **Life Sciences**
  - Better biofuels
  - Sequence to structure to function

These breakthrough scientific discoveries and facilities require multi-petaflop and beyond applications and resources.

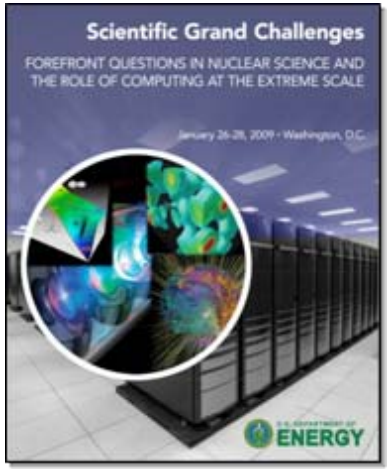
Hubble image of lensing

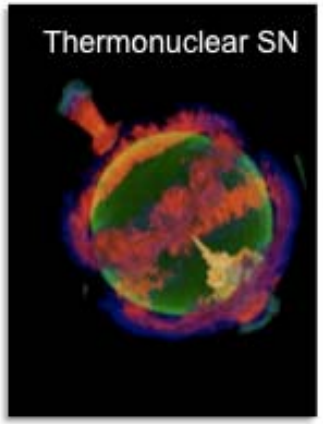






Structure of nucleons





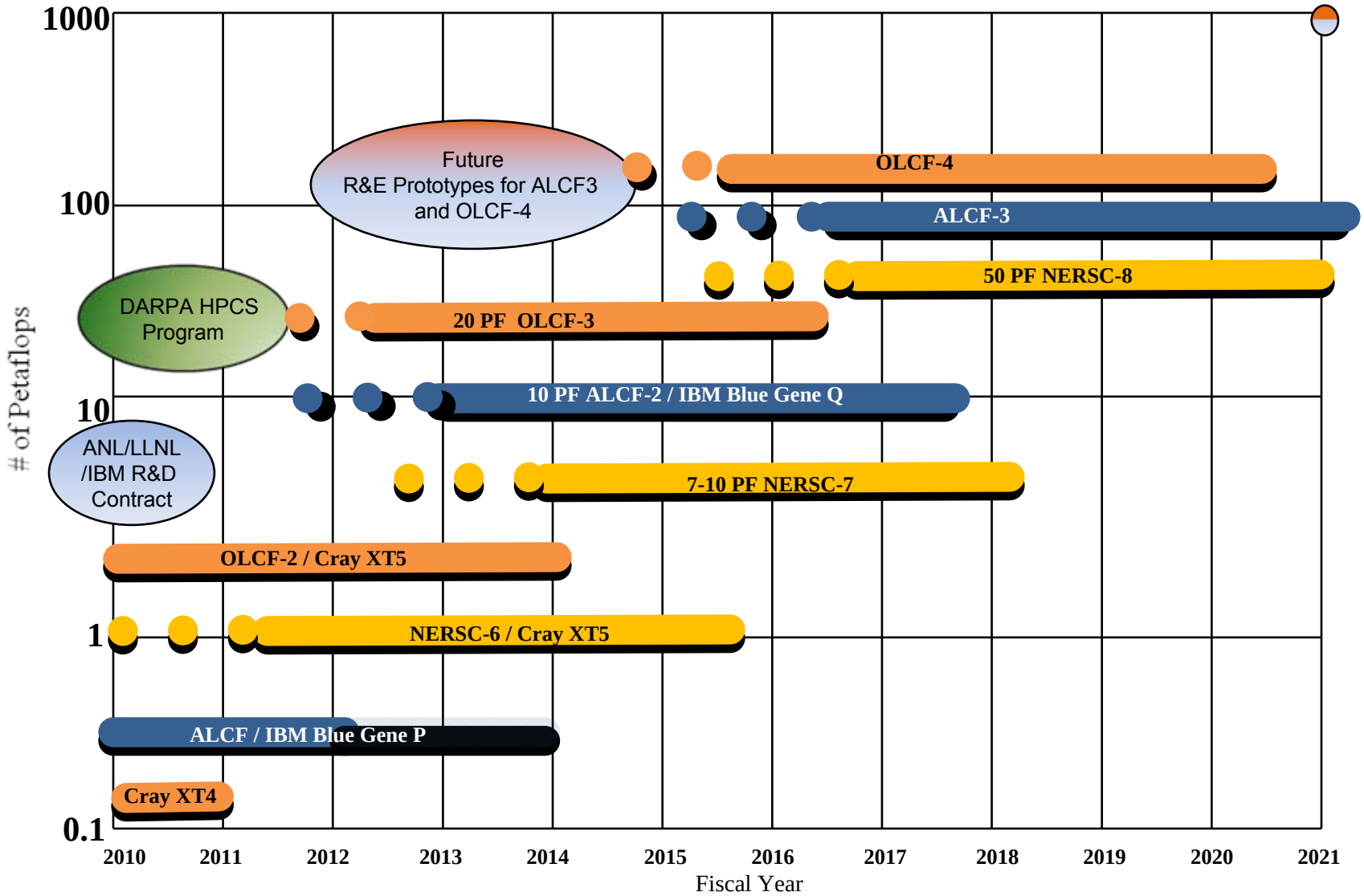
Vision for SciDAC Tomorrow

Bridging Center and Institutes

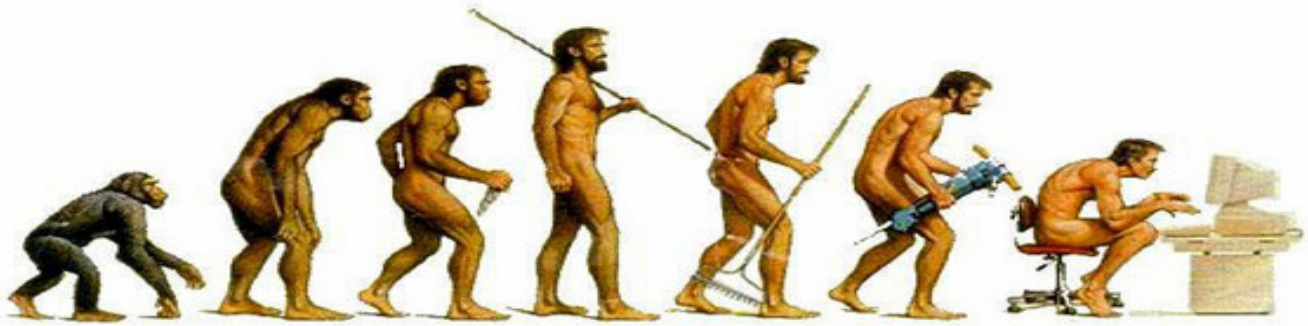
- **Reaching out to young investigators:**
  - Early Career Research Program – 2009
    - 369 Applications Received for ASCR application areas: Applied Mathematics, Computer Science, Computational Science Applications, Network Environment Research
    - 7 awards
      - **Youssef Marzouk**, Massachusetts Institute of Technology, Applied Math (Uncertainty, Stochastic and Complex Systems)
      - **Anil Vullikanti**, Virginia Polytechnic Institute and State University, Applied Math (Data and Discrete System Analysis)
      - **Patrick Chiang**, Oregon State University, Computer Science (Hardware and Power Management)
      - **Michelle Strout**, Colorado State University, Computer Science (Programming Languages/ Models/Environments & Compilers)
      - **Grigory Bronevestky**, Lawrence Livermore National Laboratory, Computer Science (Operating Systems and Fault Tolerance)
      - **Kalyan Perumalla**, Oak Ridge National Laboratory, Computer Science (Programming Languages/Models/Environments and Compilers)
      - **Christiane Jablonowski**, University of Michigan, Computational Science (Climate)

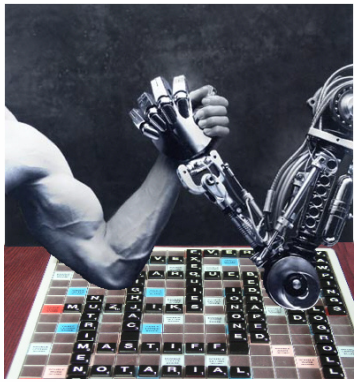
Vision for SciDAC Tomorrow

ASCR Facilities



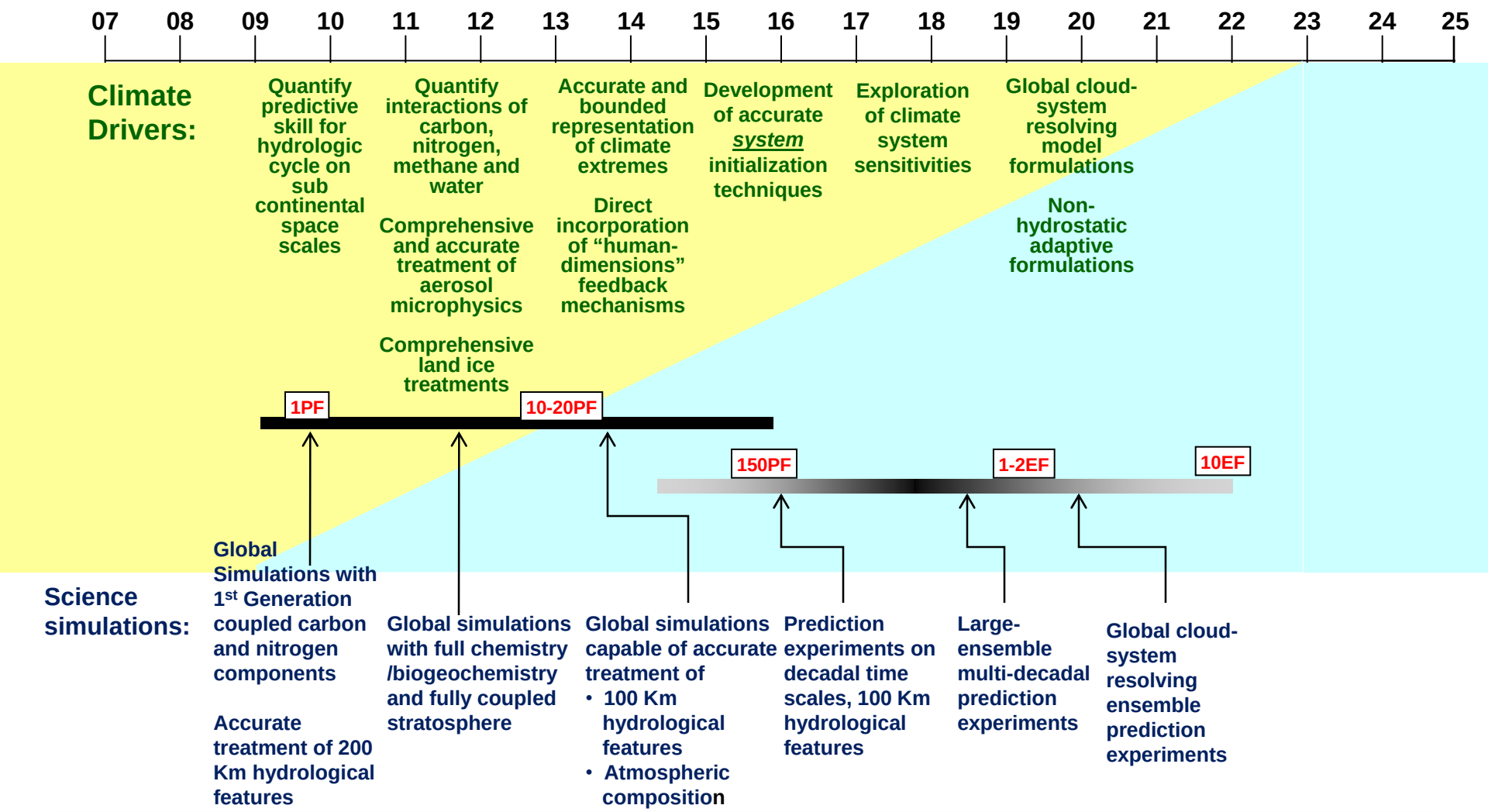
Evolution to Exascale





Gigascale — **Terascale** — Petascale — **Ex**ascale

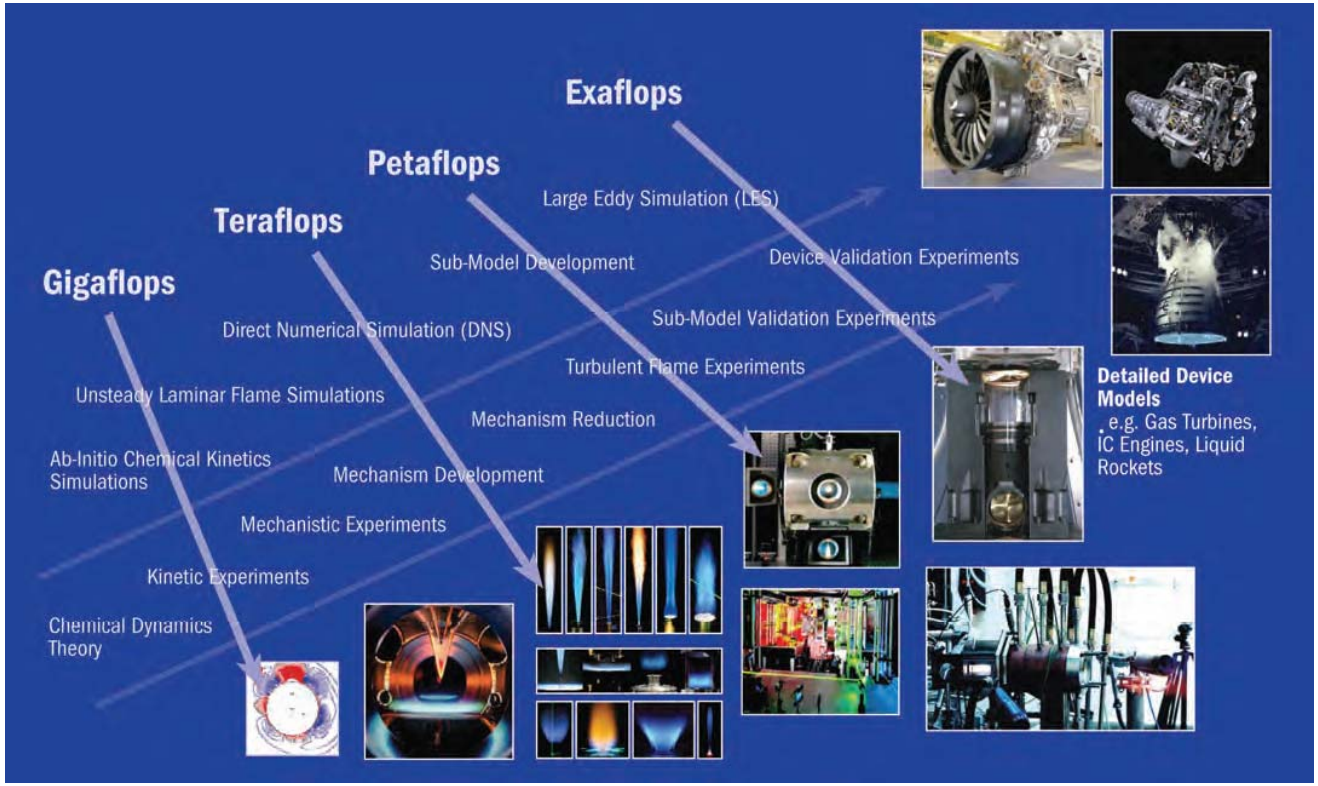
Computational science roadmap for a predictive, integrated climate model



Exascale for Energy: Combustion

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.



The road to exascale will enable robust simulations in this important area and will directly impact US competitiveness, jobs, the economy, and the policy landscape.

Geologic Carbon Sequestration

Single Injection Site
- Moderate-resolution flow + heat transport
- Low-resolution flow + heat transport + geochemistry + geomechanics

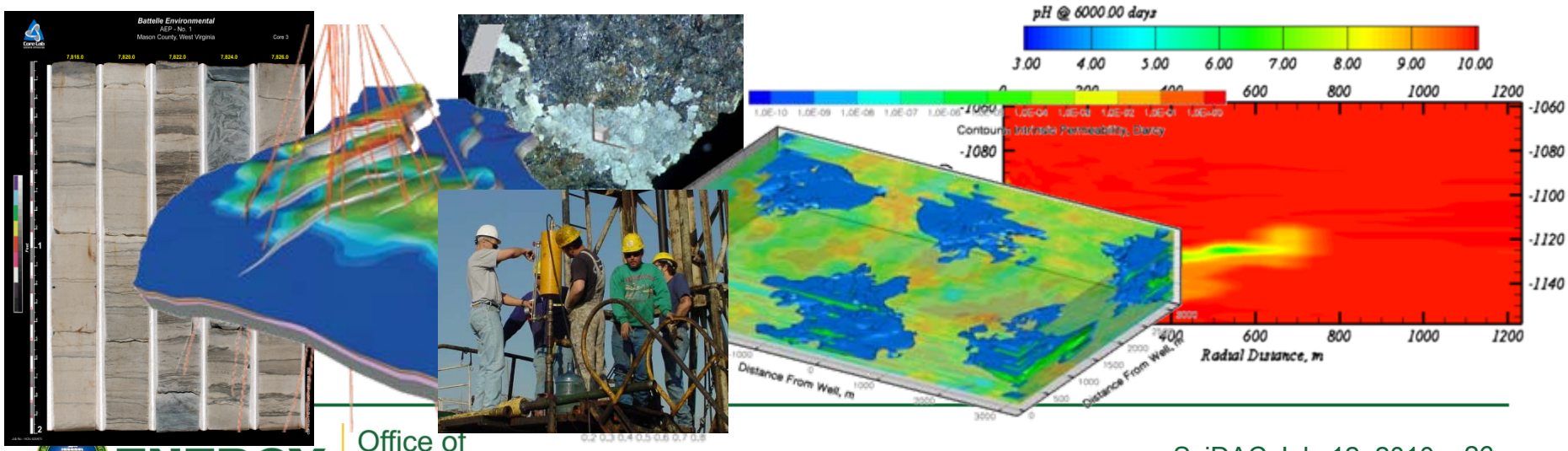
Basin-Scale Injection
- Moderate-resolution flow + heat transport
- Low-resolution flow + heat transport + geochemistry + geomechanics

Basin-Scale Injection
- High-resolution flow + heat transport
- Moderate-resolution flow + heat transport + geochemistry + geomechanics

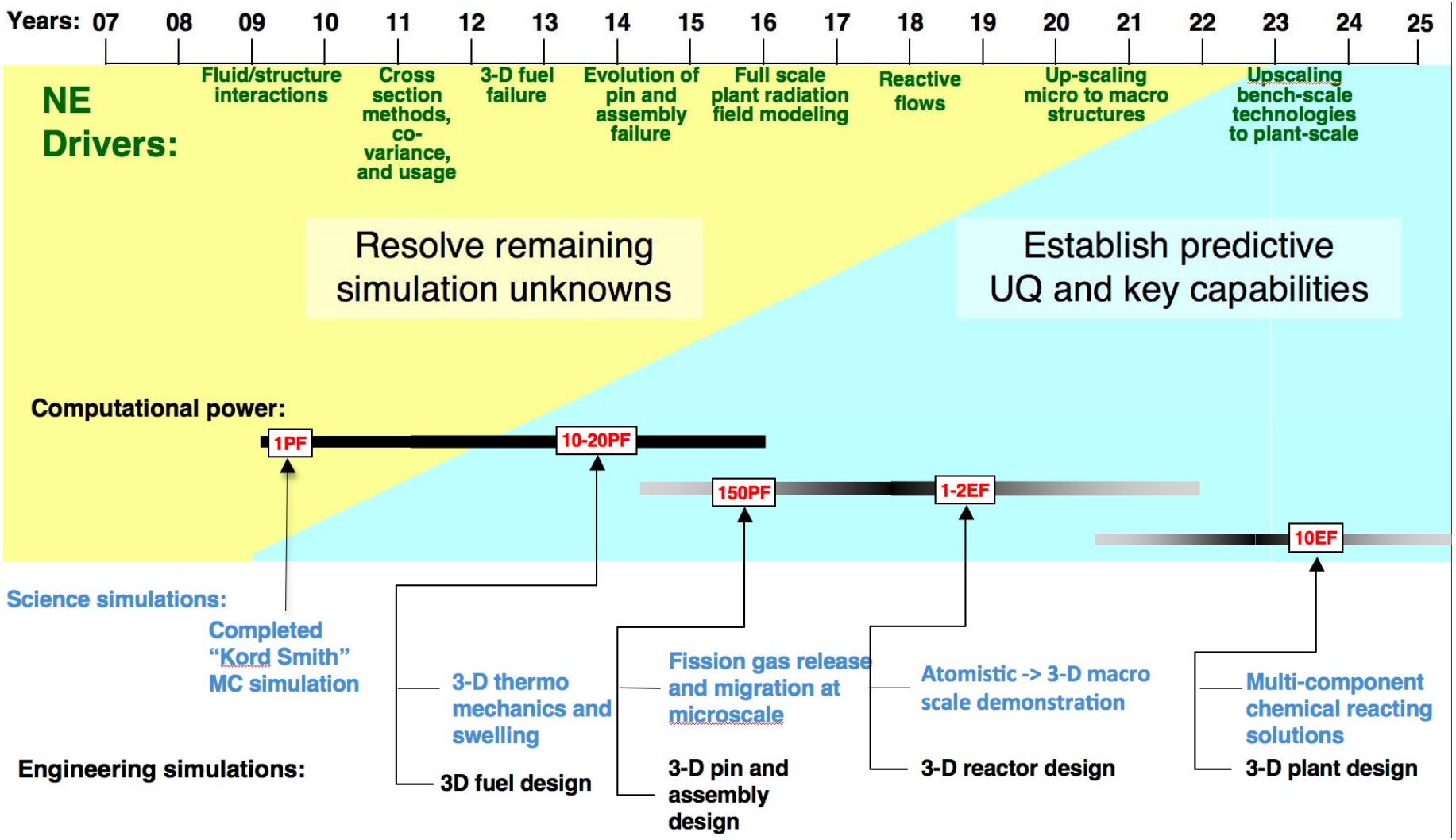
Multi-Scale Models
- Coupled pore-scale and continuum-scale modeling
- Coupled subsurface and atmospheric modeling

Gigascale — Terascale — Petascale — Exascale

Increasing grid resolution and coupled process complexity



Computational science road map
Predictive integrated modeling of nuclear systems



Exascale ≠ Petascale X 1000

- **Traditionally, PDE-based applications have expected 10x increase in resolution with each 1000x increase in compute capability, *but not this time:***
  - We won't have 1000x the memory available
  - The processors won't be 10x faster
  - Proportionally, we won't be able to move as much data on or off each processor
  - Introduction of massive parallelism at the node level is a significant new challenge (MPI is only part of the solution)

- **However, exascale computing is an opportunity for…**
  - ***More Fidelity:*** Incorporate more physics instead of increased resolution
  - ***Greater Understanding:*** Develop uncertainty quantification (UQ) to establish confidence levels in computed results and deliver predictive science

Reaching for Exascale

"Is Theology Poetry?", *C.S. Lewis*

From The Weight of Glory
"It is like watching something come gradually into focus; first it hangs in the clouds of myth and ritual,vast and vague, then it condenses, grows hard and in a sense small..."

From Miracles
"The old field of space, time, matter, and the senses is to be weeded, dug, and sown for a new crop."

Steven E. Koonin

Under Secretary For Science, Department of Energy