FY 2012 Budget Request to Congress for DOE's Office of Science Advanced Scientific Computing Research

March 30, 2011

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for Advanced Scientific Computing Research
U.S. Department of Energy
science.energy.gov/ascr

Advanced Scientific Computing Research

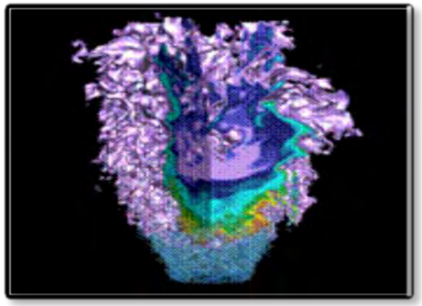
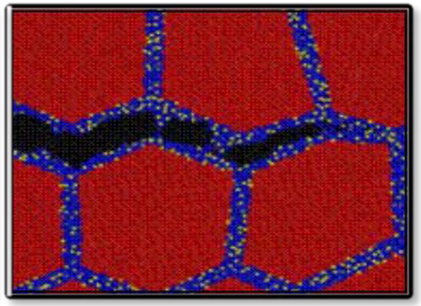
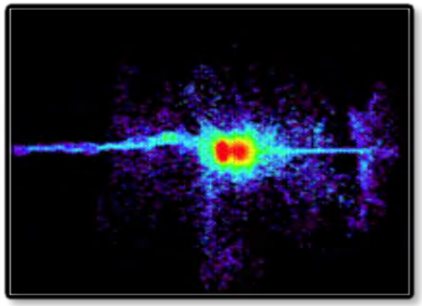
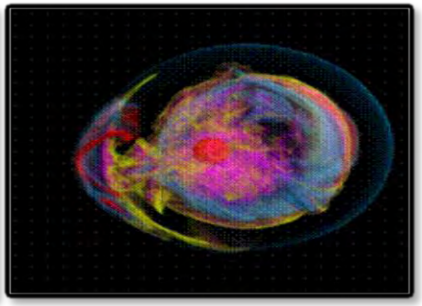
Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

The Scientific Challenges:

- Deliver next-generation scientific applications using today's petascale computers.
- Discover, develop and deploy tomorrow's exascale computing and networking capabilities.
- Develop, in partnership with U.S. industry, next generation computing hardware and tools for science.
- Discover new applied mathematics and computer science for the ultra-low power, multicore-computing future.
- Provide technological innovations for U.S. leadership in Information Technology to advance competitiveness.

FY 2012 Highlights:

- Research in uncertainty quantification for drawing predictive results from simulation
- Co-design centers to deliver next generation scientific applications by coupling application development with formulation of computer hardware architectures and system software.
- Investments in U.S. industry to address critical challenges in hardware and technologies on the path to exascale
- Installation of a 10 petaflop low-power IBM Blue Gene/Q at the Argonne Leadership Computing Facility and a hybrid, multi-core prototype computer at the Oak Ridge Leadership Computing Facility.

ASCR Budget Overview

		FY 2010 Budget	FY 2011 Request	FY 2012 Request	FY 2012 vs. FY 2010
	Advanced Scientific Computing Research				
Exascale	Applied Mathematics	43,698	45,450	48,973	+ 5,275
Exascale	Computer Science	45,936	47,400	47,400	+1,464
Exascale	Computational Partnerships (includes SciDAC)	49,538	53,297	60,036	+10,498
	Next Generation Networking for Science	14,373	14,321	12,751	-1,622
	SBIR/STTR	0	4,623	4,873	+4,873
	Total, Mathematical, Computational, and Computer Sciences Research	*153,545*	*165,091*	*174,033*	*+20,488*
	High Performance Production Computing (NERSC)	54,900	56,000	57,800	+ 2,900
	Leadership Computing Facilities	128,788	158,000	156,000	+27,212
	Research and Evaluation Prototypes	15,984	10,052	35,803	+19,819
Exascale	High Performance Network Facilities and Testbeds (ESnet)	29,982	30,000	34,500	+ 4,518
	SBIR/STTR	0	6,857	7,464	+7,464
	Total, High Performance Computing and Network Facilities	*229,654*	*260,909*	*291,567*	*+61,913*
	Total, Advanced Scientific Computing Research	**383,199[a]**	**426,000**	**465,600**	**+82,401**

- Applied Mathematics (+5,275): Supports Uncertainty Quantification ($5M)
- Computer Science (+1,464): Increases Exascale relevant research
- Computational Partnerships (+10,498): Supports Co-Design partnerships ($25M)
- Next Generation Networking for Science (-1,622): Transfers Grids to production (funding from other programs)
- NERSC (+2,900): Supports Hopper Ops
- Leadership Computing Facilities (+27,212): Supports installation of BG/Q & prototype
- Research and Evaluation Prototypes (+19,819): Supports new vendor partnerships aimed at advancing critical technologies (e.g. power management, memory, fault tolerance) ($35M)
- ESnet (+4,518): Supports planning for procurement of dedicated optical ring

[a] Total is reduced by $10,801, $9,643 of which was transferred to the Small Business Innovation Research (SBIR) program, and $1,158 of which was transferred to the Small Business Technology Transfer (STTR) program.

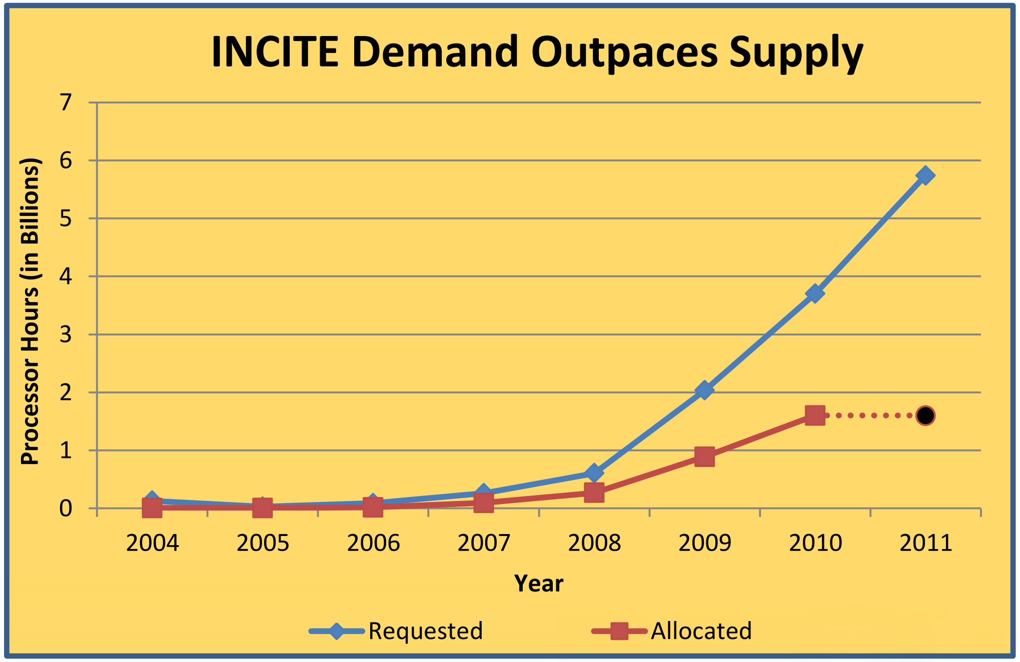
Science and Engineering at the Petascale

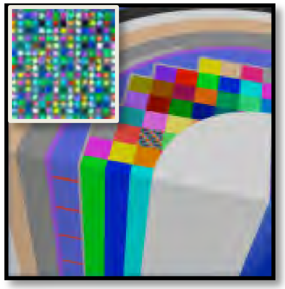
Argonne Leadership Computing Facility

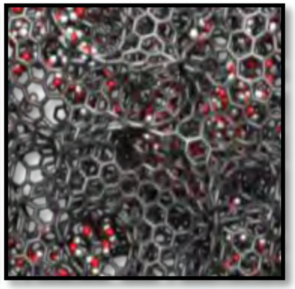
Oak Ridge Leadership Computing Facility

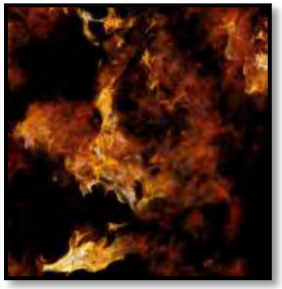
In FY 2012, the Argonne LCF will be upgraded with a 10 petaflop IBM Blue Gene/Q. The Oak Ridge LCF will continue site preparations for a system expected in FY 2013 that will be 5-10 times more capable than the Cray XT-5.

- The Cray XT5 ("Jaguar") at ORNL and the IBM Blue Gene/P ("Intrepid") at ANL will provide ~2.3 billion processor hours in FY12 to address science and engineering problems that defy traditional methods of theory and experiment and that require the most advanced computational power.
- Peer reviewed projects are chosen to advance science, speed innovation, and strengthen industrial competitiveness.
- Demand for these machines has grown each year, requiring upgrades of both.




Nuclear Reactor Simulation


Energy Storage Materials


Turbulence

Delivering Capabilities that Keep the U.S. IT Sector Competitive
"ASCR inside"

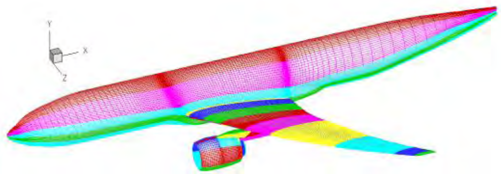
A few ASCR Technologies and the Companies that Use them

- **MPICH** – **Message passing library**
  "MPICH's impact comes from the fact that since it is open source, portable, efficient, and solid, most computer vendors have chosen it as the foundation of the MPI implementation that they supply to their customers as part of their system software." - Rusty Lusk, MPICH consortia
  ""MPICH is critical to the development of the F135 engine, which will power America's next-generation Joint Strike Fighter," - Robert Barnhardt, VP, Pratt & Whitney
- **Fastbit** – **Search algorithm for large-scale datasets**
  "FastBit is at least 10 times, in many situations 100 times, faster than current commercial database technologies" – Senior Software Engineer, Yahoo!
- **OSCARS** - **On-demand virtual network circuits**
  "It used to take three months, 13 network engineers, 250 plus e-mails and 20 international conference calls to set up an inter-continental virtual circuit. With OSCARS and collaborative projects, we can establish this link in 10 minutes." - Chin Guok, ESnet network engineer
- ***perfSONAR*** - **network performance monitoring**
  "These tools give us better visibility into the network, allowing us to troubleshoot performance issues quickly."
  -- Internet2 Network Performance Workshop participant

Delivering INCITE – Computing Facilities Contribute to U.S. Competitiveness

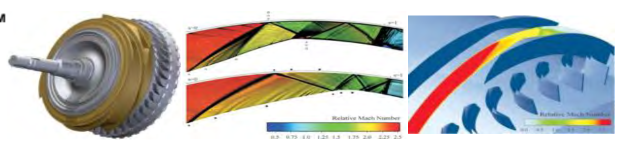
U.S. DEPARTMENT OF ENERGY | Office of Science

- Smart Truck Brands went from concept to design to manufacturer in 18 months.
- Demonstrated fuel mileage improvements of 7% to 12% available 2011. Exceeds California CARB requirements.



- Boeing demonstrated the effectiveness and accuracy of high fidelity computational fluid dynamics simulation tools and then used them in designing their next generation of aircraft.
- Significantly reduced the need for costly physical prototyping and wind tunnel testing. Accelerated airplane design and lowered cost.

- GE determined the effects of unsteady flow interactions between blade rows on the efficiency of highly loaded turbines.
- Provided design engineers with the analytical tools to extract greater design efficiency and fuel savings.

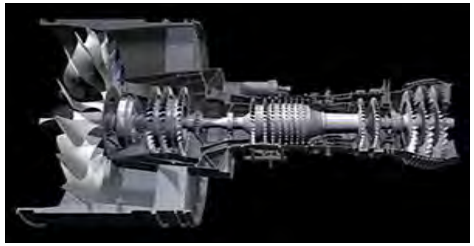


- Ramgen used computational fluid dynamics with shock compression to expedite design-cycle analysis, and to make large stage configuration analyses possible.
- Advanced the development curve of the CO_2 compressor with next generation rotor now scheduled for testing in February 2012.

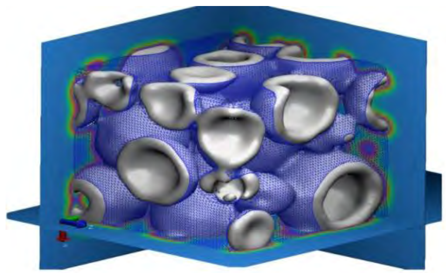
- Accelerate materials research by at least a year to help GM meet fuel economy and emissions standards.
- A prototype thermoelectric generator in a Chevy Suburban generated up to 5% improvement in fuel economy.

- UT studies of nickel and platinum are demonstrating that the less expensive nickel can be used as a catalyst to produce hydrogen.

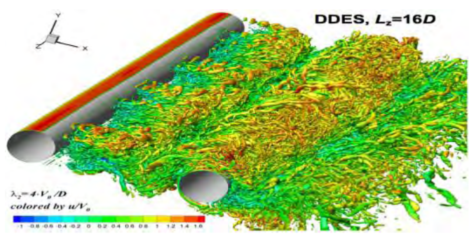
Delivering INCITE – Computing Facilities Contribute to U.S. Competitiveness



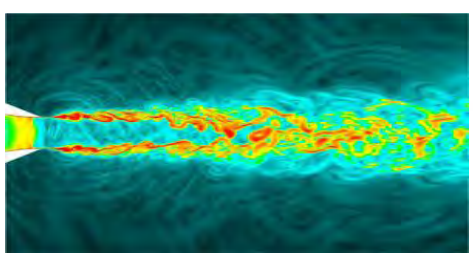
- Pratt and Whitney using "virtual testing" to accelerate improvements in jet engine design, dramatically decreasing problem-solution turnaround times in development of PurePower™ engine.
- The new-generation engine improves fuel burn by 12-15%, with a potential savings to airlines of nearly $1M per aircraft per year. It also cuts carbon emissions by 3,000 tons per aircraft per year while reducing other emissions 50%.



- P&G was able to study the complex interactions of billions of atoms and create simulations to determine how tiny submicroscopic structures impact the characteristics of the ingredients in soaps, detergents, lotions and shampoos.
- Understanding these processes accelerates the development of many consumer goods, foods, and fire control materials.



- Boeing simulated the turbulence created by aircraft landing gear and calculated the noise caused by two cylinders placed in tandem in an air stream. This uses state of the art turbulence-resolving CFD for massively separated flows.
- Boeing expects these capabilities to contribute to the design of safe and quiet technologies.



- GE Global Research simulated the complex turbulent flows that generate aerodynamic noise during takeoff to validate the accuracy of a large eddy simulation solver.
- The simulations are considered by GE to be critical for developing next-generation, "green" (low-emission) aircraft.

Broadening Our Impact – Working with the Council on Competitiveness

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Compete. Council on Competitiveness

High Performance Computing
Case Study.
Procter & Gamble's Story of Suds, Soaps, Simulations and Supercomputers

High Performance Computing
Advance.
Benchmarking Industrial Use of High Performance Computing for Innovation

High Performance Computing
Case Study.
Lighting Up DreamWorks with High Performance Computing

High Performance Computing
Case Study.
Boeing Catches a Lift with High Performance Computing

Public-Private Partnerships for Leveraging U.S. HPC Expertise
May 13, 2010

Contents

U.S. Manufacturing— Global Leadership Through Modeling and Simulation
White Paper
4 March 2009

This is today's headline: *The Collapse of Manufacturing*, and many U.S. manufacturers and their supply chains are in crisis. In this time of crisis, the U.S. has the technological tools to maintain our competitive edge and global leadership in manufacturing, but we risk our manufacturing leadership position if we fail to ... game-changing tool of high performance computing (HPC) for modeling, simulation, and analysis.

ASCR Outreach Workshop with Independent Software Vendors*
Scheduled for
March 31, 2011
in Chicago, IL
outreach.scidac.gov/industry_software/

**The majority of U.S. ISVs are small businesses*

Investments for Exascale Computing

Opportunities to Accelerate the Frontiers of Science through HPC

Why Exascale?

- Science:
  Computation and simulation advance knowledge in science, energy, and national security; numerous S&T communities and Federal Advisory groups have demonstrated the need for computing power 1,000 times greater than we have today.

- U.S. Leadership:
  The U.S. has been a leader in high performance computing for decades. U.S. researchers benefit from open access to advanced computing facilities, software, and programming tools.

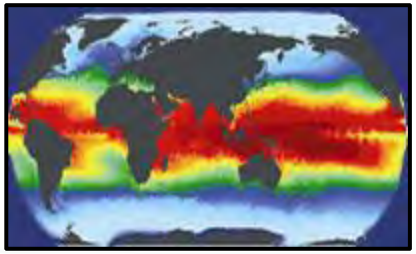
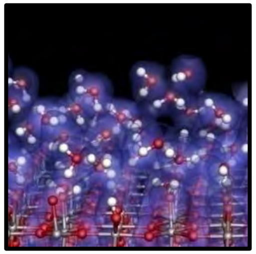
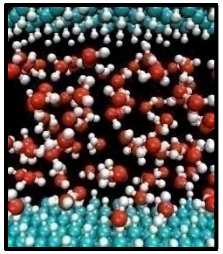
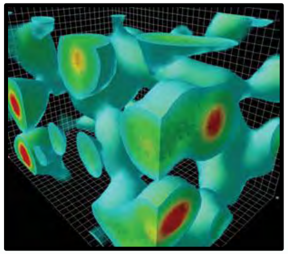
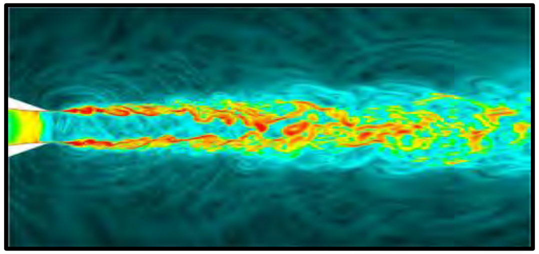
- Broad Impact:
  Achieving the power efficiency, reliability, and programmability goals for exascale will have dramatic impacts on computing at all scales–from PCs to mid-range computing and beyond.

DOE Activities will:

- Build on Success
  DOE delivered Petascale science and engineering– Firmly re-establishing U.S. leadership in Computational Science.

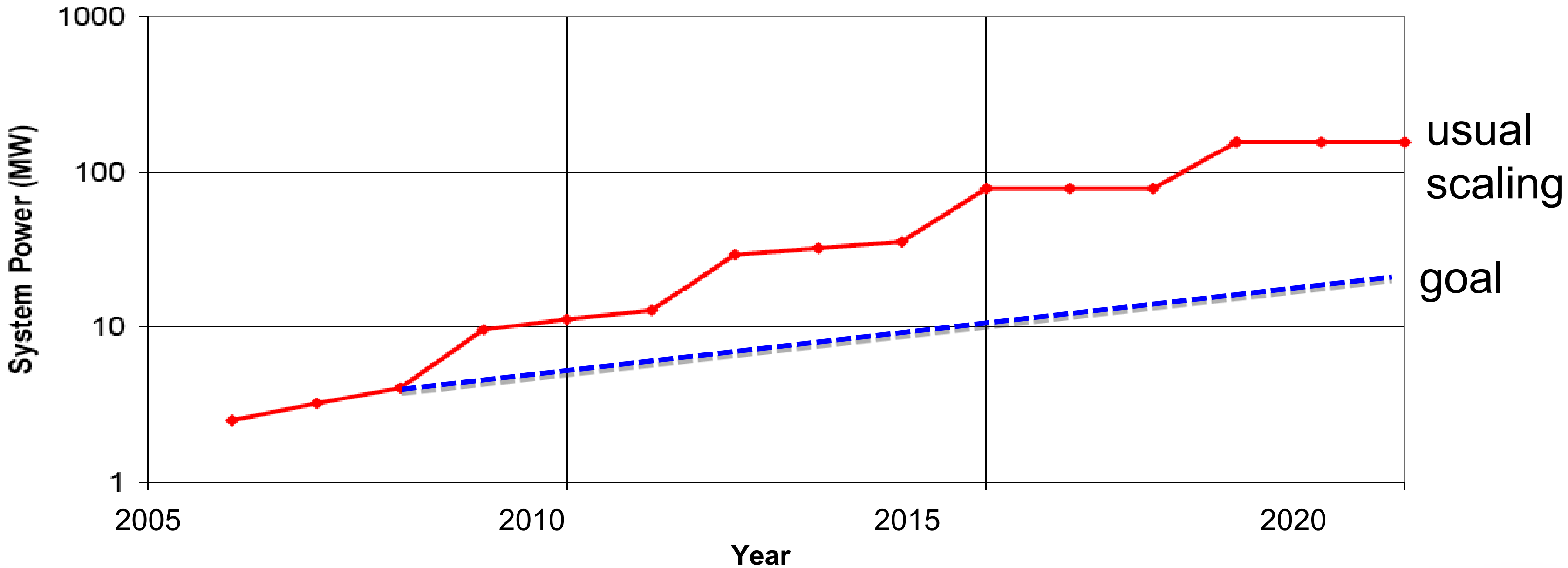
- Use What Works – Co-design
  The embedded computing industry realized that it was not a significantly large market force to ensure that "off the shelf" offerings met their specific needs. They adopted a co-design partnership with vendors to great success. DOE will copy this successful approach since scientific computing is also a small part of the overall computing market.

- Focus on What Matters Most
  – Partner with Vendors on Grand Challenges– this will also enable U.S. manufacturers to leapfrog foreign competition.
  – Use "mission-critical" Department of Energy Applications as part of the Co-design process – also ensures a broad spectrum of applications will be ready for Exascale.

Exascale is about Energy Efficient Computing

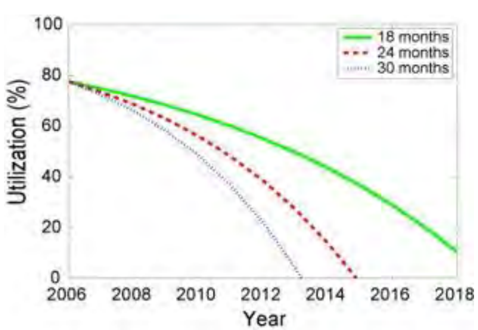
- **At $1M per MW, energy costs are substantial**
- **1 petaflop in 2010 will use 3 MW**
- **1 exaflop in 2018 at 200 MW with "usual" scaling**
- **1 exaflop in 2018 at 20 MW is target**



Three Grand Challenges
that Must be Solved to Delivering Exascale Computing

- **Energy Utilization**
  - An Exascale machine built from today's technology would take more than a gigawatt of electricity or the output of a small modular nuclear reactor.
  - Memory and data movement are the key energy hogs.

- **Parallelism in the Extreme (Concurrency)**
  - Billions of regular processors and specialized processors need to work together and share data seamlessly without moving the data very often.



Projections of effective application utilization in future HPC systems under checkpoint restart model

- **Fault Tolerance**
  - An Exascale machine built from today's technology would operate for only a few minutes at a time due to chip failures.
  - For such a computer to be useful, the mean failure rate must be measured in days or weeks.

Solving these Grand Challenges would reap rewards across the U.S. IT sector and across science and engineering – from petaflop desktops to exaflops

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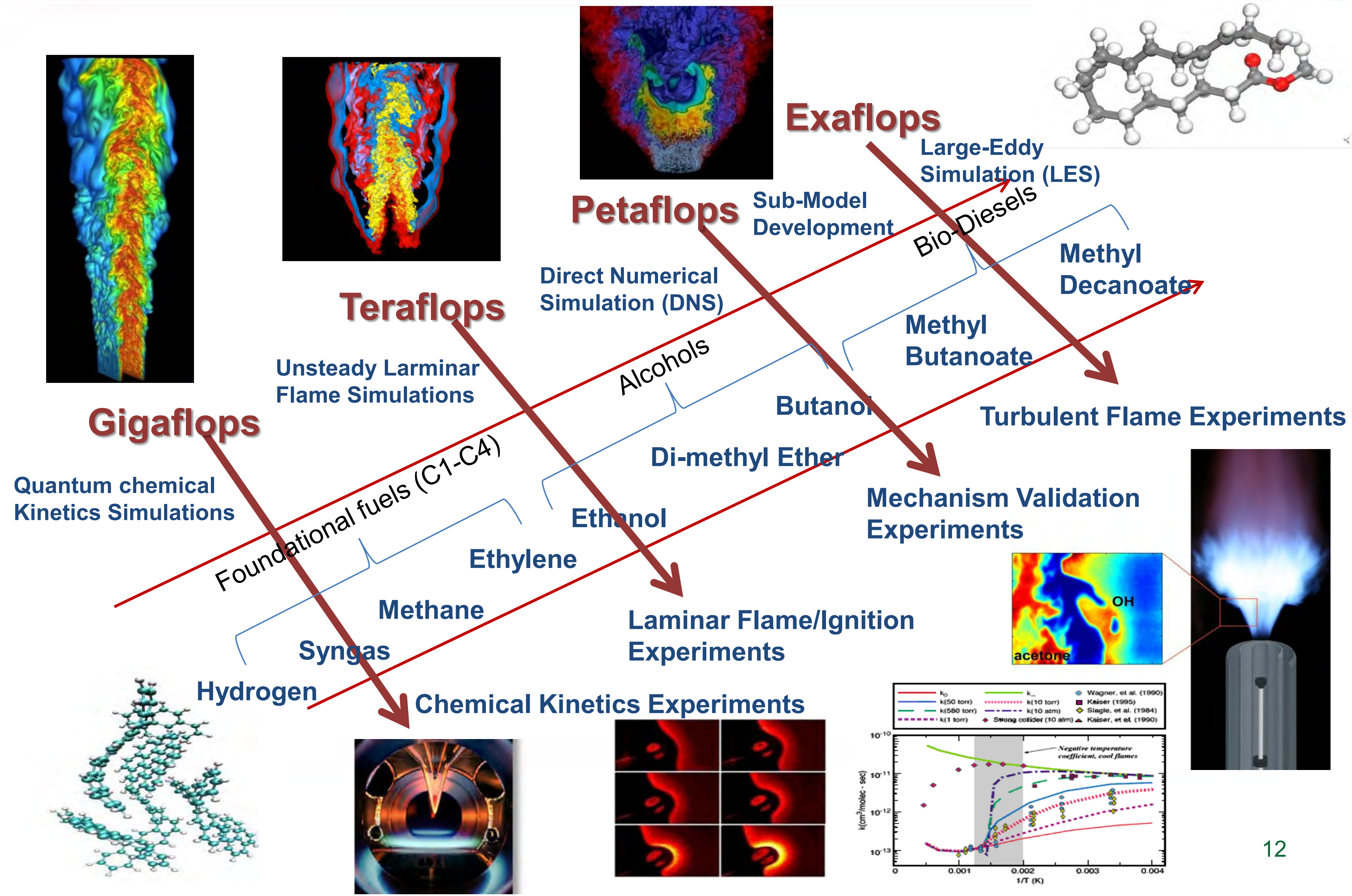
Why Exascale?

Combustion Models Coupling Biofuels with Turbulence



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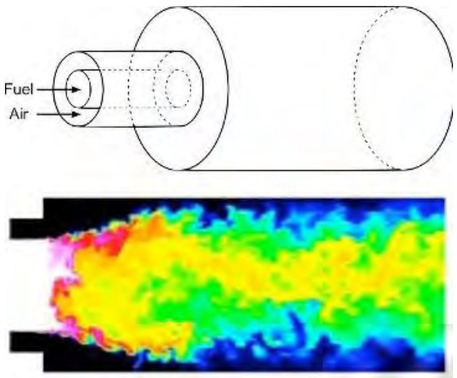
Why Exascale

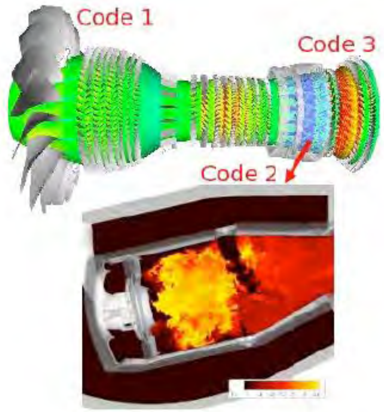
Improving Safety, Fuel Efficiency, and Competitiveness

Terascale
State-of-the-art in 1997



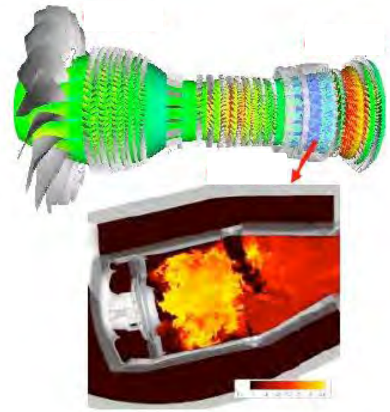
Shown are a schematic (top) of a coaxial combustor with air-methane co-flow and an instantaneous snapshot of the mixture fraction (bottom) from the first LES of turbulent combustion in a research combustor performed at Stanford University. The simulations used a flamelet and progress-variable approach with over two million degrees of freedom computed on the ASCI Red platform at Sandia National Laboratories. Note that the highest-fidelity simulations of reactive flow in 1997 were restricted to simple geometries and gas-phase only physics.

Petascale
State-of-the-art in 2007



Comprehensive simulation of the flow through an entire jet engine performed by Stanford University, under the NNSA ASCI Program, and Pratt & Whitney. The compressor (Code 1) and the turbine (Code 3) were computed using RANS while the combustor (Code 2) used LES. Data is transferred across these interfaces using a coupled, multi-code, multi-physics integration environment. Contours of entropy in the compressor and turbine sections are shown while the flame in the combustor is visualized via contours of temperature in a mid-plane section from a realistic PW6000 engine.

Exascale
State-of-the-art in 201?



One multi-scale, first principles, code to optimize designs with alternative fuel chemistry in advanced engine designs

The current industry standard simulation tools have plateaued in their ability to resolve the critical technical challenges that arise as the operability and performance thresholds of aerospace vehicle and jet engines are driven to their limits. A new suite of first-principles, simulation-based engineering design tools must become a standard component in the engineering design cycle. This increased level of simulation fidelity has the potential to expand the current design envelope, eschew industrial stagnation and augment human creativity with first-principles, simulation-based engineering science tools.

"The key finding of the Panel is that there are compelling needs for exascale computing capability to support the DOE's missions in energy, national security, fundamental sciences, and the environment. The DOE has the necessary assets to initiate a program that would accelerate the development of such capability to meet its own needs and by so doing benefit other national interests." - Trivelpiece Panel Report, January, 2010

"Exascale computing will uniquely provide knowledge leading to transformative advances for our economy, security and society in general. A failure to proceed with appropriate speed risks losing competitiveness in information technology, in our industrial base writ large, and in leading-edge science." - Advanced Scientific Computing Advisory Committee

Exascale Progress

- **Proposals processed in Exascale related topic areas:**
  - Applied Math: Uncertainty Quantification
  - Computer Science: Advanced Architectures
  - Computer Science: X-Stack
  - Computer Science: Data Management and Analysis at Extreme Scales
  - Computational Partnerships: Co-Design
- **Exascale Coordination with DOD and DARPA**
- **Close Collaboration with NNSA**
  - Weekly leadership calls
  - Program mangers exchanges
  - Coordinated PI meetings
  - Management plan and MOU

Summary

- The FY 2012 budget supports activities needed for delivering petascale science today and meeting the challenges of hybrid, multi-core computing for predictive exascale science and engineering in the next decade.
  - Critical to continued leadership in computational science
  - Critical for continued U.S. leadership in Information Technology
  - Success will have wide reaching impacts across the U.S. IT sector, High-tech Industry and science and engineering
- Office of Science computing and networking needs will be met.
- Begins expanding benefits of high performance computational science and engineering to the DOE applied programs.

ASCR at a Glance

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Relevant Websites

ASCR: science.energy.gov/ascr/
ASCR Workshops and Conferences:
science.energy.gov/ascr/news-and-resources/workshops-and-conferences/
SciDAC: www.scidac.gov
INCITE: science.energy.gov/ascr/facilities/incite/
Exascale Software: www.exascale.org
DOE Grants and Contracts info: science.doe.gov/grants/

Backup

Why Exascale
Applications and Technology Challenges

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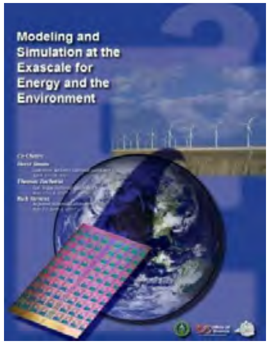
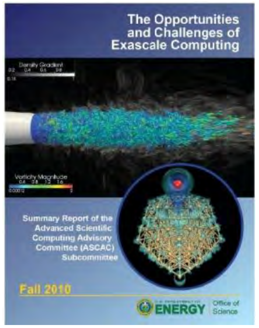
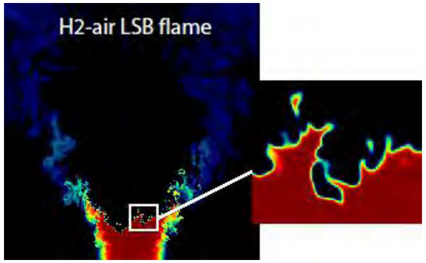
http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/grand-challenges/

- **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**
  - Trivelpiece Panel (1/10)
  - ASCAC Exascale Charge (FACA) (11/10)







MISSION IMPERATIVES

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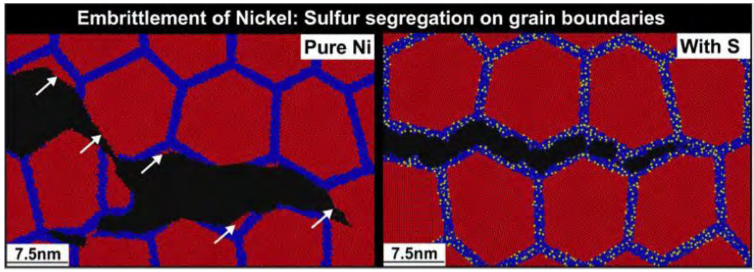
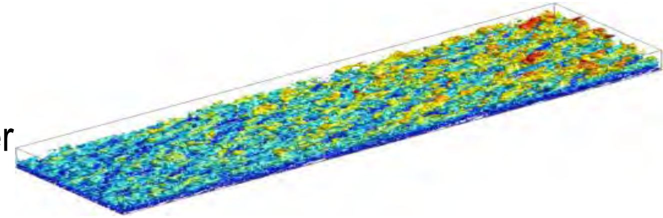
ASCR Computational Research Delivers Public Benefits – Saving Energy

Stress Corrosion Cracking - Priya Vashishta, USC



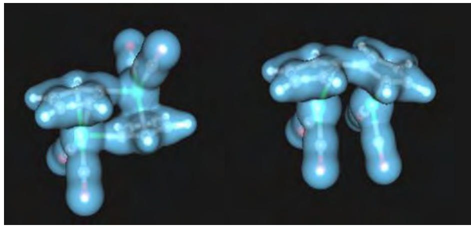
- Annually, corrosion costs about $276 Billion (3% of GDP).
- Performance and lifetime of materials in nuclear and advanced power generation are severely limited by corrosion from extreme conditions.
- Simulations link sulfur impurities and embrittlement of Nickel.

Turbulence - Robert Moser, *UT-Austin*

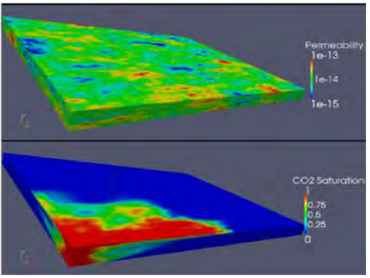


- 20% of world energy consumption (100 quadrillion BTU) due to turbulence.
- Virtual redesign reduces costly drag on piping, ducts, and vehicles.
- Simulations show where viscous near-wall turbulence interacts with outer-layer resulting in energy losses in transport of fuels in pipes and flow past vehicles.

Storing Solar Energy - Jeffrey Grossman, MIT

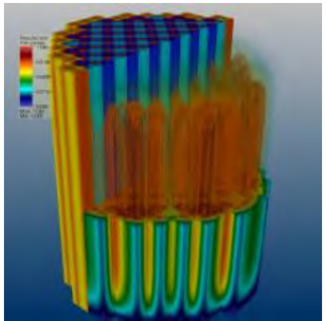


- Capturing solar energy in chemical form can make it storable and transportable.
- Simulations reveal how *fulvalene diruthenium* molecules change configuration when they absorb heat from sunlight informing the search for similar, less expensive compounds



Subsurface – Mary Wheeler, University of Texas at Austin

- High fidelity models of complex geosystems are key tools for groundwater remediation, sequestration of carbon in saline aquifers and enhanced petroleum production.
- Simulations have been used to characterize the US Eagle Ford shale formations in collaboration with industrial partners Chevron, IBM, and ConocoPhillips.



NE Modeling and Simulation Hub (CASL) - Doug Kothe, *Oak Ridge Nat. Lab.*

- 20% of U.S. electricity comes from Nuclear.
- NE Modeling and Simulation Hub builds on numerous ASCR developed capabilities and tools.