U.S. DEPARTMENT OF ENERGY | Office of Science

View from Germantown

March 26, 2012

Dr. Daniel Hitchcock
Associate Director for Advanced Scientific Computing Research
U.S. Department of Energy
www.science.energy.gov

Advanced Scientific Computing Research

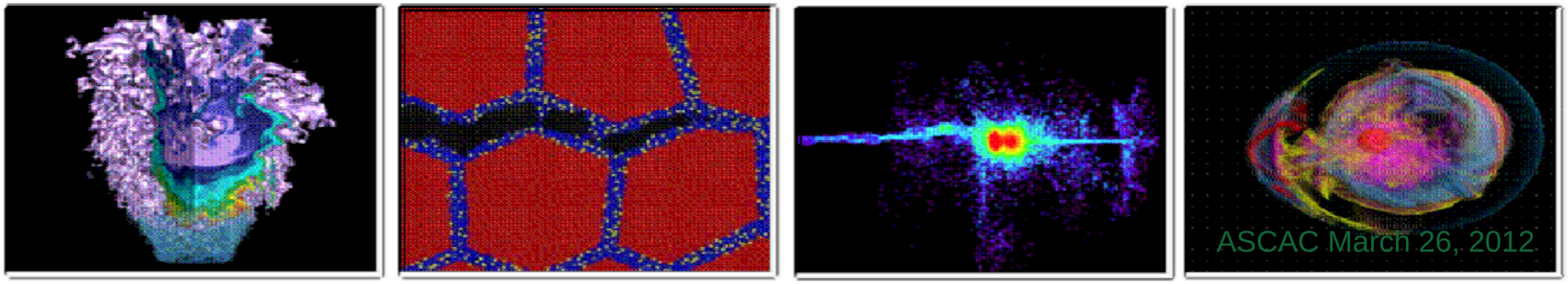
Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

The Scientific Challenges:

- Deliver next-generation scientific and energy applications on multi-petaflop computers.
- Discover, develop and deploy exascale computing and networking capabilities.
- Partner with U.S. industry to develop the next generation computing hardware and tools for science.
- Discover new applied mathematics, computer science, and networking tools for the ultra-low power, multicore-computing future and data-intensive science.
- Provide technological innovations for U.S. leadership in Information Technology to advance competitiveness.

FY 2013 Highlights:

- Co-design centers to deliver next generation scientific applications.
- Investments with U.S. industry to address critical challenges on the path to exascale.
- Operation of a 10 petaflop low-power IBM Blue Gene/Q at the Argonne Leadership Computing Facility and installation and early science access to a hybrid, multi-core computer at the Oak Ridge Leadership Computing Facility.
- **Research efforts across the portfolio in support of data-intensive science including the massive data produced by Scientific User Facilities.**



ASCR Budget Overview

		FY 2011 Budget	FY 2012 Enacted	FY 2013 Request	FY 2013 vs. FY 2012	
	Advanced Scientific Computing Research					
Exascale Big Data	Applied Mathematics	45,604	45,604	49,500	+ 3,896	Math for data-intensive science
Exascale Big Data	Computer Science	47,301	47,400	54,580	+ 7,180	Computer Science challenge of big data
Exascale Big Data	Computational Partnerships (includes SciDAC)	52,813	44,250	56,776	+ 12,526	Co-design center and partnerships for data-intensive science
Big Data	Next Generation Networking for Science	12,313	12,751	16,194	+ 3,443	Networking challenges of data-intensive science
	SBIR/STTR	0	4,560	5,570	+ 1,010	
	Total, Mathematical, Computational, and Computer Sciences Research	*158,031*	*154,565*	*182,620*	*+28,055*	
	High Performance Production Computing (NERSC)	59,514	57,800	65,605	+ 7,805	Supports site prep. for new NERSC bld.
	Leadership Computing Facilities	158,020	156,000	145,000	-11,000	Reduce infrastructure investments
Exascale	Research and Evaluation Prototypes	4,301	30,000	22,500	- 7,500	Focus vendor partnerships and critical technologies
	High Performance Network Facilities and Testbeds (ESnet)	30,451	34,500	32,000	- 2,500	Supports staged production deployment of 100Gbps optical ring
	SBIR/STTR	0	8,003	7,868	- 135	
	Total, High Performance Computing and Network Facilities	*252,286*	*286,303*	*272,973*	*-13,330*	
	Total, Advanced Scientific Computing Research	**410,317**	**440,868**	**455,593**	**+14,725**	

[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.

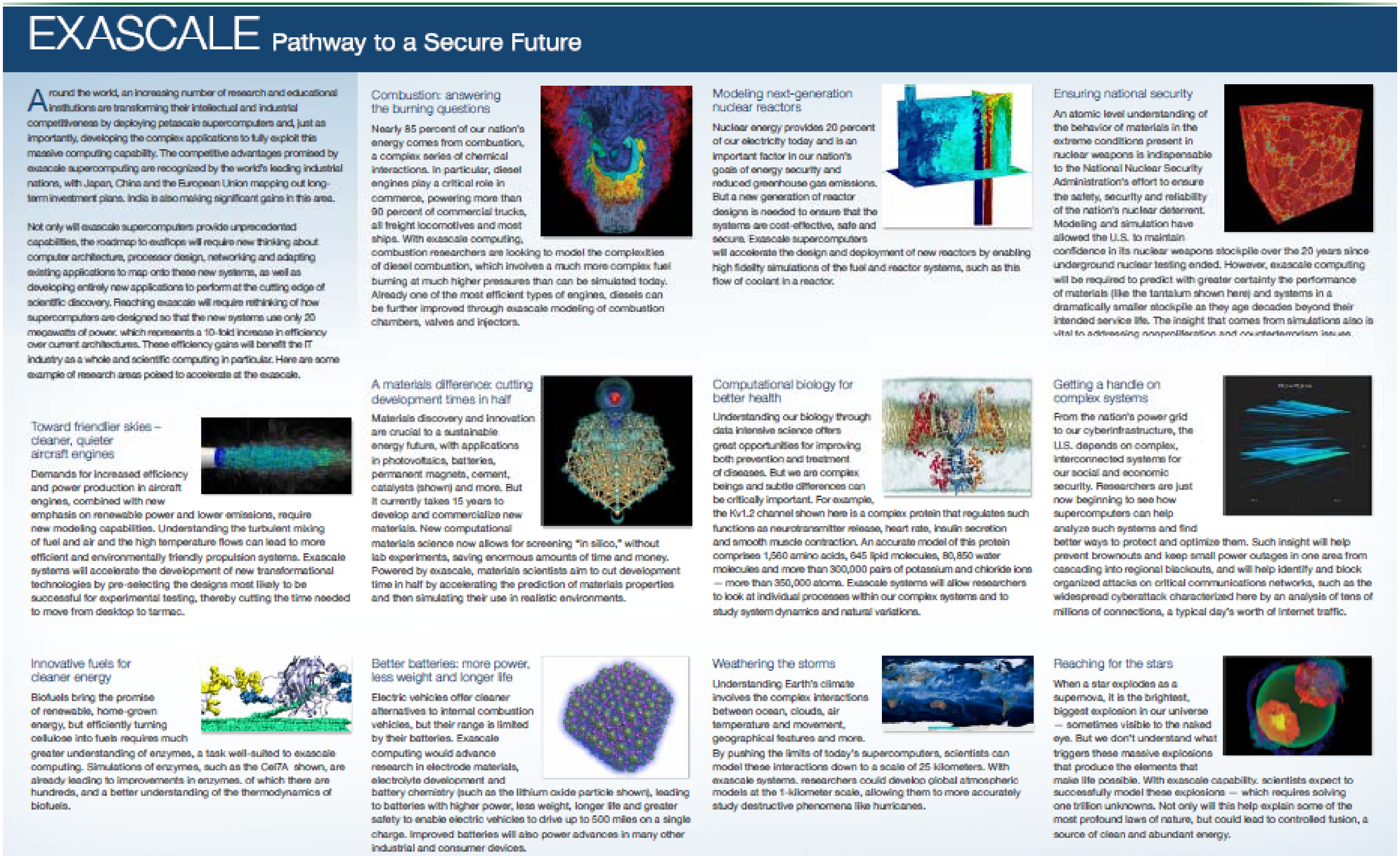
ASCR Personnel News

- Facilities Division Director Position Open

  http://www.usajobs.gov/GetJob/ViewDetails/311382800

  Position Closes April 9, 2012
- Hope to have openings this summer for Computer Science, Computational Mathematics, and Facilities Management.

Why Exascale



EXASCALE Pathway to a Secure Future

Around the world, an increasing number of research and educational institutions are transforming their intellectual and industrial competitiveness by deploying petascale supercomputers and, just as importantly, developing the complex applications to fully exploit this massive computing capability. The competitive advantages promised by exascale supercomputing are recognized by the world's leading industrial nations, with Japan, China and the European Union mapping out long-term investment plans. India is also making significant gains in this area.

Not only will exascale supercomputers provide unprecedented capabilities, the roadmap to exaflops will require new thinking about computer architecture, processor design, networking and adapting existing applications to map onto these new systems, as well as developing entirely new applications to perform at the cutting edge of scientific discovery. Reaching exascale will require rethinking of how supercomputers are designed so that the new systems use only 20 megawatts of power, which represents a 10-fold increase in efficiency over current architectures. These efficiency gains will benefit the IT industry as a whole and scientific computing in particular. Here are some example of research areas poised to accelerate at the exascale.

Toward friendlier skies – cleaner, quieter aircraft engines

Demands for increased efficiency and power production in aircraft engines, combined with new emphasis on renewable power and lower emissions, require new modeling capabilities. Understanding the turbulent mixing of fuel and air and the high temperature flows can lead to more efficient and environmentally friendly propulsion systems. Exascale systems will accelerate the development of new transformational technologies by pre-selecting the designs most likely to be successful for experimental testing, thereby cutting the time needed to move from desktop to tarmac.

Innovative fuels for cleaner energy

Biofuels bring the promise of renewable, home-grown energy, but efficiently turning cellulose into fuels requires much greater understanding of enzymes, a task well-suited to exascale computing. Simulations of enzymes, such as the Cel7A shown, are already leading to improvements in enzymes, of which there are hundreds, and a better understanding of the thermodynamics of biofuels.

Combustion: answering the burning questions

Nearly 85 percent of our nation's energy comes from combustion, a complex series of chemical interactions. In particular, diesel engines play a critical role in commerce, powering more than 90 percent of commercial trucks, all freight locomotives and most ships. With exascale computing, combustion researchers are looking to model the complexities of diesel combustion, which involves a much more complex fuel burning at much higher pressures than can be simulated today. Already one of the most efficient types of engines, diesels can be further improved through exascale modeling of combustion chambers, valves and injectors.

A materials difference: cutting development times in half

Materials discovery and innovation are crucial to a sustainable energy future, with applications in photovoltaics, batteries, permanent magnets, cement, catalysts (shown) and more. But it currently takes 15 years to develop and commercialize new materials. New computational materials science now allows for screening "in silico," without lab experiments, saving enormous amounts of time and money. Powered by exascale, materials scientists aim to cut development time in half by accelerating the prediction of materials properties and then simulating their use in realistic environments.

Better batteries: more power, less weight and longer life

Electric vehicles offer cleaner alternatives to internal combustion vehicles, but their range is limited by their batteries. Exascale computing would advance research in electrode materials, electrolyte development and battery chemistry (such as the lithium oxide particle shown), leading to batteries with higher power, less weight, longer life and greater safety to enable electric vehicles to drive up to 500 miles on a single charge. Improved batteries will also power advances in many other industrial and consumer devices.

Modeling next-generation nuclear reactors

Nuclear energy provides 20 percent of our electricity today and is an important factor in our nation's goals of energy security and reduced greenhouse gas emissions. But a new generation of reactor designs is needed to ensure that the systems are cost-effective, safe and secure. Exascale supercomputers will accelerate the design and deployment of new reactors by enabling high fidelity simulations of the fuel and reactor systems, such as this flow of coolant in a reactor.

Computational biology for better health

Understanding our biology through data intensive science offers great opportunities for improving both prevention and treatment of diseases. But we are complex beings and subtle differences can be critically important. For example, the Kv1.2 channel shown here is a complex protein that regulates such functions as neurotransmitter release, heart rate, insulin secretion and smooth muscle contraction. An accurate model of this protein comprises 1,560 amino acids, 645 lipid molecules, 80,850 water molecules and more than 300,000 pairs of potassium and chloride ions — more than 350,000 atoms. Exascale systems will allow researchers to look at individual processes within our complex systems and to study system dynamics and natural variations.

Weathering the storms

Understanding Earth's climate involves the complex interactions between ocean, clouds, air temperature and movement, geographical features and more. By pushing the limits of today's supercomputers, scientists can model these interactions down to a scale of 25 kilometers. With exascale systems, researchers could develop global atmospheric models at the 1-kilometer scale, allowing them to more accurately study destructive phenomena like hurricanes.

Ensuring national security

An atomic level understanding of the behavior of materials in the extreme conditions present in nuclear weapons is indispensable to the National Nuclear Security Administration's effort to ensure the safety, security and reliability of the nation's nuclear deterrent. Modeling and simulation have allowed the U.S. to maintain confidence in its nuclear weapons stockpile over the 20 years since underground nuclear testing ended. However, exascale computing will be required to predict with greater certainty the performance of materials (like the tantalum shown here) and systems in a dramatically smaller stockpile as they age decades beyond their intended service life. The insight that comes from simulations also is vital to addressing nonproliferation and counterterrorism issues.

Getting a handle on complex systems

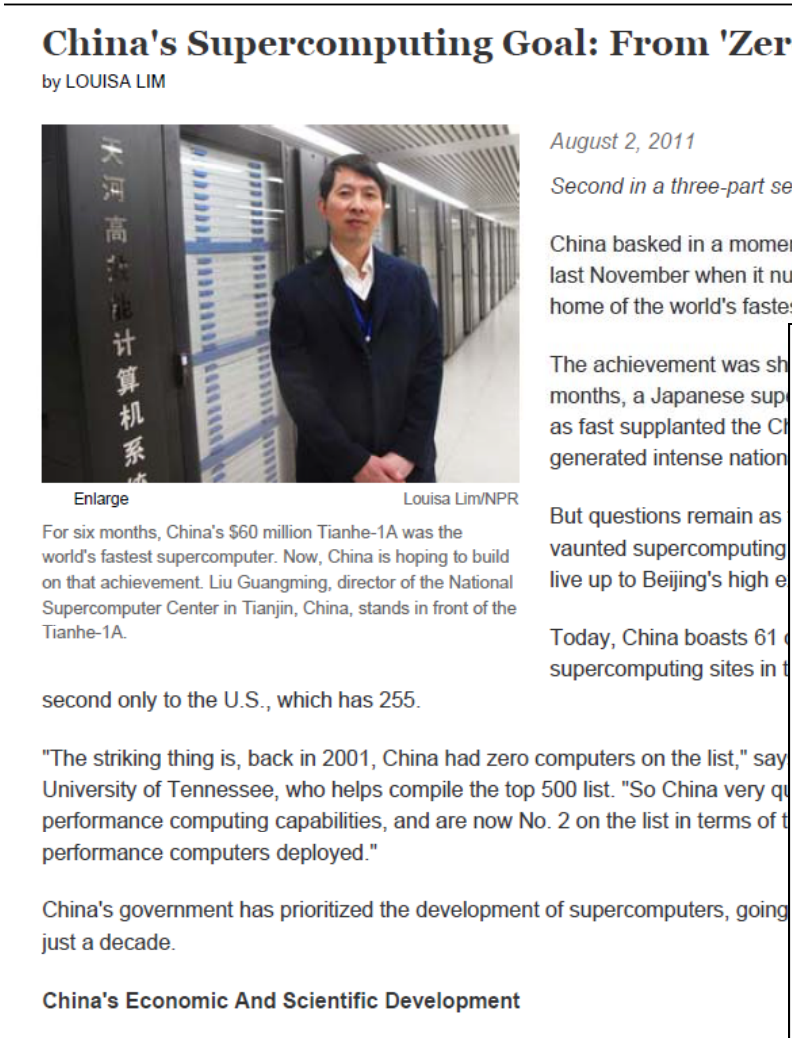
From the nation's power grid to our cyberinfrastructure, the U.S. depends on complex, interconnected systems for our social and economic security. Researchers are just now beginning to see how supercomputers can help analyze such systems and find better ways to protect and optimize them. Such insight will help prevent brownouts and keep small power outages in one area from cascading into regional blackouts, and will help identify and block organized attacks on critical communications networks, such as the widespread cyberattack characterized here by an analysis of tens of millions of connections, a typical day's worth of Internet traffic.

Reaching for the stars

When a star explodes as a supernova, it is the brightest, biggest explosion in our universe — sometimes visible to the naked eye. But we don't understand what triggers these massive explosions that produce the elements that make life possible. With exascale capability, scientists expect to successfully model these explosions — which requires solving one trillion unknowns. Not only will this help explain some of the most profound laws of nature, but could lead to controlled fusion, a source of clean and abundant energy.

International Recognition of Importance of Exascale

But exascale systems "pose numerous hard challenges," said the European Commission (EC) in a report that accompanied its funding announcements. The challenges include 100-fold reduction in energy consumption along with development of new programming models. As Europe sees it, solving these challenges creates opportunity for Europe, China and others looking to take on U.S. HPC dominance.



China's Supercomputing Goal: From 'Zero To Hero'

by LOUISA LIM

August 2, 2011

Second in a three-part series

Enlarge Louisa Lim/NPR

For six months, China's $60 million Tianhe-1A was the world's fastest supercomputer. Now, China is hoping to build on that achievement. Liu Guangming, director of the National Supercomputer Center in Tianjin, China, stands in front of the Tianhe-1A.

China basked in a moment of technological glor last November when it nudged out the U.S. as home of the world's fastest supercomputer.

The achievement was sh months, a Japanese sup as fast supplanted the Cl generated intense nation

But questions remain as vaunted supercomputing live up to Beijing's high e

Today, China boasts 61 c supercomputing sites in t second only to the U.S., which has 255.

"The striking thing is, back in 2001, China had zero computers on the list," say University of Tennessee, who helps compile the top 500 list. "So China very qu performance computing capabilities, and are now No. 2 on the list in terms of t performance computers deployed."

China's government has prioritized the development of supercomputers, going just a decade.

China's Economic And Scientific Development

COMPUTERWORLD

Europe plans exascale funding above U.S. levels

White House budget for exascale offers 'peanuts for U.S. effort

Patrick Thibodeau

February 21, 2012 (Computerworld)

By Patrick Thibodeau Secretariat was famous for coming up from behind in a race to win, and the same may be true for the U.S. in the global push to build exascale technologies. Because for now, when it comes to delivering the needed funding to build these systems, the U.S. is just getting out of the gate.

The European Commission last week said it is doubling its investment in the push for

February 16, 2012

Europe Aims to Become World Leader in Supercomputing

Michael Feldman

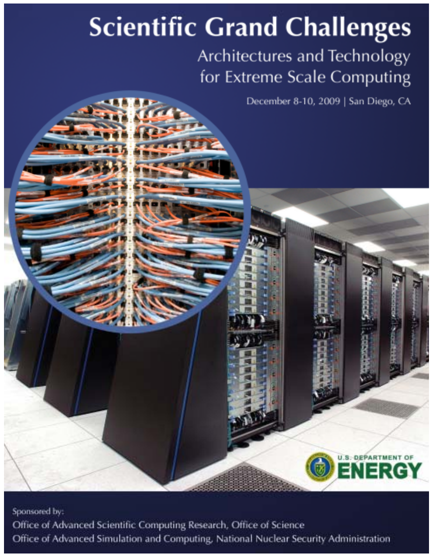
In what is increasingly seen as a global competition for supercomputing capability, the European Commission (EC) this week put forth a plan (http://www.hpcwire.com/hpcwire/2012-02-15/eurpean_commission_announces_plan_to_double_hpc_investments.html) to double its investment in high performance computing and deploy exascale machines before the end of the decade. The plan would increase Europe's public HPC spend from €630 million to €1.2 billion and pump a greater share of the money into development, training, and creating "new centres of excellence."

Some of the impetus to crank up supercomputing investment by the Europeans is being driven by the globalization of the technology. That world-wide competition they face is reflected by the build-out of supercomputing infrastructure across the world. For example, three years ago, the US owned 58 percent of the fastest supercomputers, according to the TOP500 list. Today, that figure is down to 53 percent. Most of the shrinking US share was the result of the rapid growth in top supercomputers in China, which grew from 3 percent of

Partnership with NNSA

- MOU April 12, 2011
- Numerous Exascale Workshops and joint PI meetings
- Regular program manager meetings
- Accomplishment

(ASCR) *High Performance Computations Save DOE Time and Money.* A SciDAC partnership with NNSA focused on nuclear structure provided a quantitative description of neutron-tritium scattering that was precise enough for designers at the National Ignition Facility (NIF) to make critical fuel assembly decisions that could not have been achieved using physical testing within the NIF cost and schedule baselines.



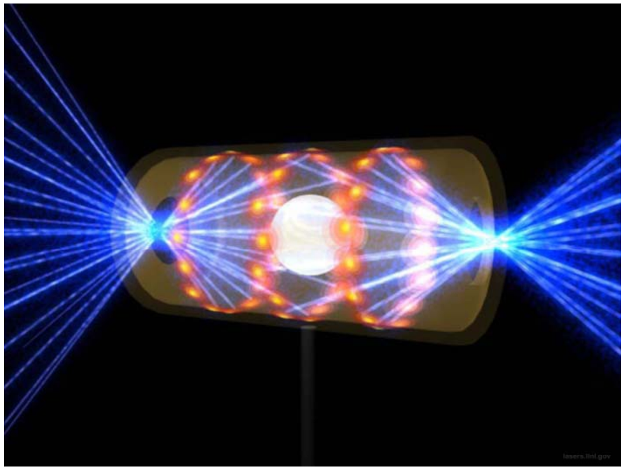
Scientific Grand Challenges

Architectures and Technology
for Extreme Scale Computing

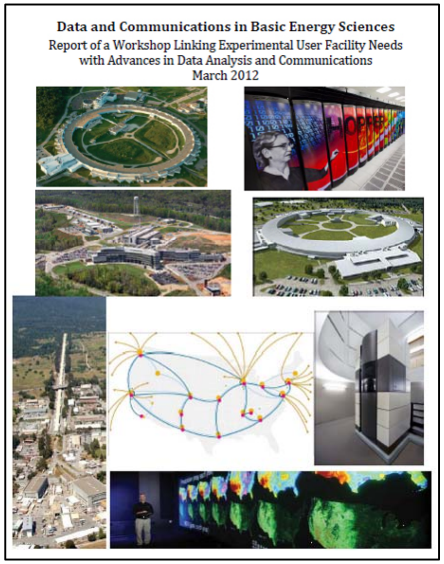
December 8-10, 2009 | San Diego, CA

U.S. DEPARTMENT OF ENERGY

Sponsored by:
Office of Advanced Scientific Computing Research, Office of Science
Office of Advanced Simulation and Computing, National Nuclear Security Administration



Why Data?



Data and Communications in Basic Energy Sciences
Report of a Workshop Linking Experimental User Facility Needs with Advances in Data Analysis and Communications
March 2012

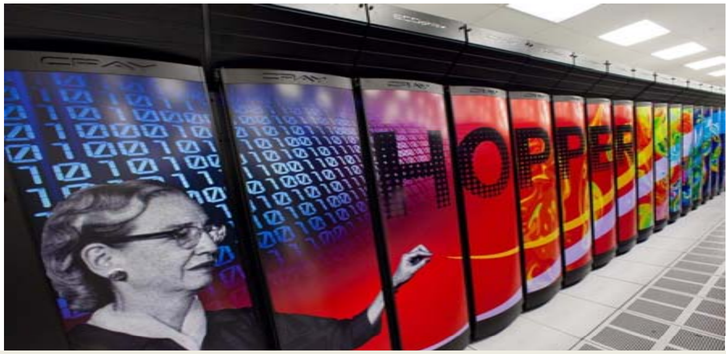
- All of the exascale hardware trends impact intensive science(in many cases more than intensive applications);
- Leverages investments in exascale to maximize impact on the Science missions;
- Data from instruments still on 18-24 month doubling because detectors on CMOS feature size path;
- Significant hardware infrastructure needed to support this which probably will not be replicated at users' home institution (i.e. launching a petabyte file transfer at a user's laptop is not friendly); and
- Responds to recommendations in December 2010 report of the President's Council of Advisors on Science and Technology - *Designing a Digital Future: Federally Funded Research and Development in Networking and Information Technology* .

http://www.whitehouse.gov/administration/eop/ostp/pcast/docsreports

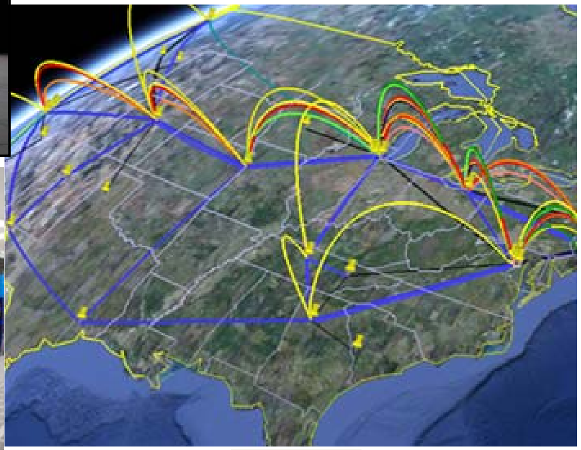
ASCR Facilities

- Providing the Facility **– High-End and Leadership Computing**
- Investing in the Future **- Research and Evaluation Prototypes**
- Linking it all together **– Energy Sciences Network (ESnet)**

Oak Ridge Leadership Computing Facility



National Energy Research Scientific Computing Center



ESnet

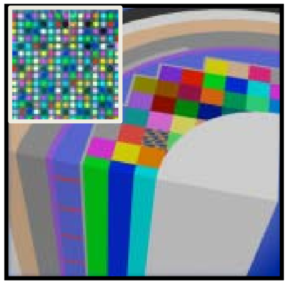
Argonne Leadership Computing Facility

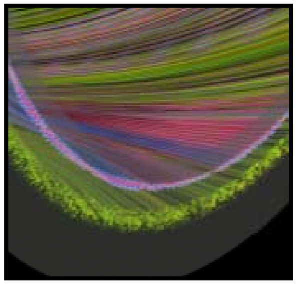
Leadership Computing Facilities Support Scientific Research for a Clean Energy Future

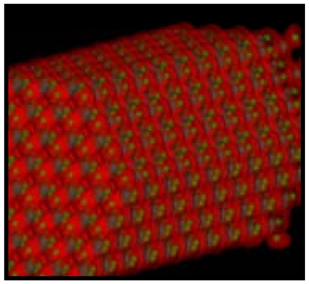
- Leadership Computing Facilities (LCF)
  - Request supports Oak Ridge LCF upgrade to 10 -20 petaflops and full operations.
    - Oak Ridge LCF decreased from FY12 to support other priorities.
    - This one time reduction was possible because of decision to upgrade in place, deferred infrastructure investment, and other infrastructure investments planned for FY13 and moved up to FY12.
  - Request supports Argonne LCF upgrade to 10 petaflops and full operations.
    - Increased to support lease payments and operating costs for 10 petaflop machine.

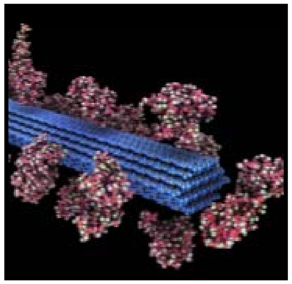
- The Cray XK6 ("Jaguar") at ORNL and the IBM Blue Gene/Q (“Mira") at ANL will provide ~3.5 billion processor hours in FY 2013 (INCITE, ALCC and Testing). Demand for these machines has grown each year, requiring upgrades of both.

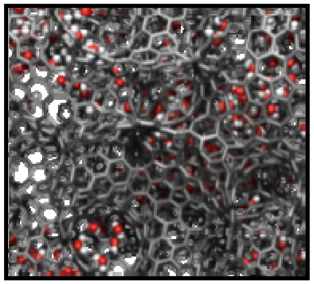
- Peer reviewed projects are chosen to advance science, speed innovation, and strengthen industrial competitiveness. Among the topics in FY2013:
  - Advancing materials for lithium air batteries, solar cells, and superconductors
  - Exploring carbon sequestration
  - Improving combustion in fuel-efficient, near-zero-emissions systems
  - Understanding how turbulence affects the efficiency of aircraft and other transportation systems
  - Designing next-generation nuclear reactors and fuels and extending the life of aging reactors


Nuclear Reactor Simulation


Fusion Plasmas


Nanoscale Science


Biofuels


Energy Storage Materials


Turbulence

2013 INCITE proposal writing webinar announcement

- "INCITE Proposal Writing Lecture/Webinars."

  March 26: http://www.olcf.ornl.gov/event/2013-incite-proposal-writing-webinar

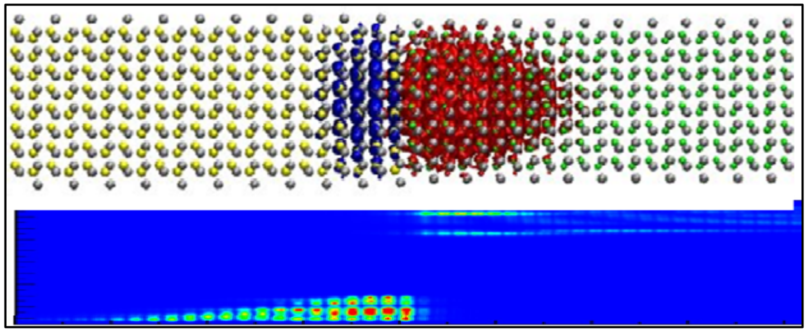
  April 24: https://www.alcf.anl.gov/incite2013
- The session will provide both prospective and returning users the opportunity to get specific answers to questions about the proposal and review process for INCITE.
- The 2013 INCITE Call for Proposals is for awards of compute time on the Cray XK6 (Titan) system at the OLCF and the IBM Blue Gene/P (Intrepid) and IBM Blue Gene/Q (Mira) systems at the ALCF.
- For more information about the INCITE program, see http://www.DOEleadershipcomputing.org

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Jaguar supercomputer helps researchers trap the power of sunlight

Three-year project aims to increase solar-cell efficiency on the atomic scale

- An ORNL supercomputer is helping scientists simulate a process leaves do naturally—capturing sunlight and turning it into energy.
- LBNL's Lin-Wang Wang and his fellow LBNL collaborator, Michael Banda, are using the OLCF's Jaguar to improve the efficiency of photovoltaics by learning more about electrically conductive material on an atomic scale.
- Today's nanostructured solar panels are only 3 to 4 percent efficient; but if nanotechnology can improve, it may be the path to cheaper solar energy.
- The team received a 3-year allocation (2010–2012) on Jaguar through the INCITE program and was awarded 10 million processor hours on Jaguar for 2011.
- The research duo's primary motivation is making solar energy a practical source of power for the masses.



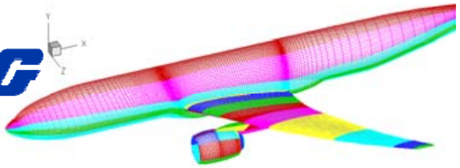
A simulation of an exciton in a cadmium selenide and cadmium telluride joint nanorod (upper panel). The blue surface shows the shape of the holes; the red surface, the shape of the electrons; and the grey, yellow, and green spheres, cadmium, selenium, and tellurium atoms, respectively. The color contour plots (lower panel) represent the existence of hole quantum states (left) and electron quantum states (right) at different energies. Image courtesy of Lin-Wang Wang, Lawrence Berkeley National Laboratory

"With a small group of computer cores to calculate each fragment and a straightforward strategy for parallelization, we can scale the computation very well to the larger number of cores on supercomputers." Co-PI Lin-Wang Wang

INCITE Computing Contributes to U.S. Competitiveness and Clean Energy

- **GE** determined the effects of unsteady flow interactions between blade rows on the efficiency of turbines.
  - Provided engineers with the analytical tools to extract greater design efficiency and fuel savings.
  - Results provided substantial ROI justification for GE to purchase its own Cray supercomputer

- **Ramgen** used computational fluid dynamics with shock compression to expedite design-cycle analysis.
  - Accelerated the development of the CO_2 compressor allowing Ramgen to go from computer design and testing to cutting a Titanium prototype in 2 months.



- **Boeing** demonstrated the effectiveness and accuracy of computational fluid dynamics simulation tools and used them in designing their next generation of aircraft.
  - Significantly reduced the need for prototyping and wind tunnel testing.

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

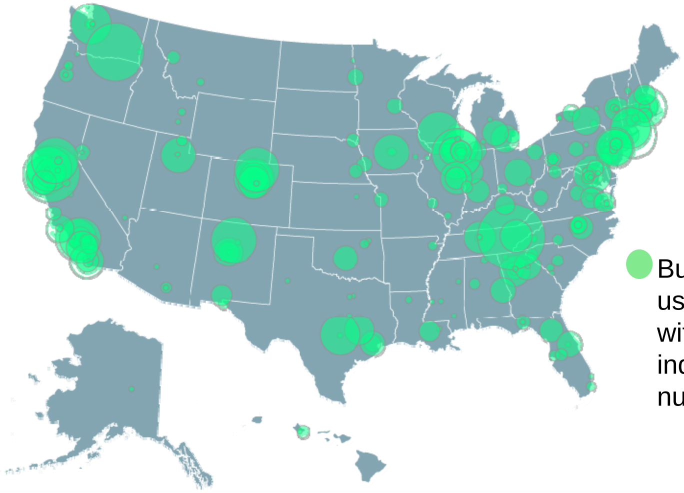
- **United Technologies** studies of nickel and platinum are demonstrating that the less expensive nickel can be used as a catalyst to produce hydrogen.

National Energy Research Scientific Computing Facility (NERSC)

Rendering of New Computation, Research, and Theory (CRT) building (view from Chu Road)

- FY13 Increase (+$7.8M) supports site preparations for planned move to a new facility on LBNL campus.
- Provides more than a petaflop of scientific computing capability for SC research community.
- Supports approximately 4,000 scientists working on 500 research projects
- Mission Need (CD-0) for NERSC-7 signed February 10, 2012

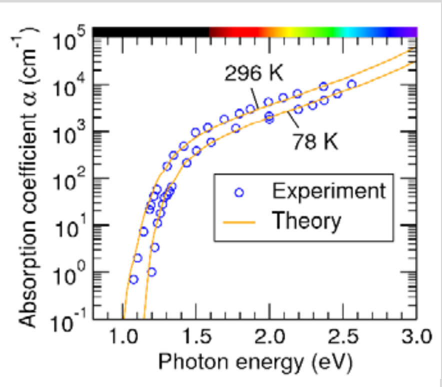
NERSC Extramural Users FY 2011



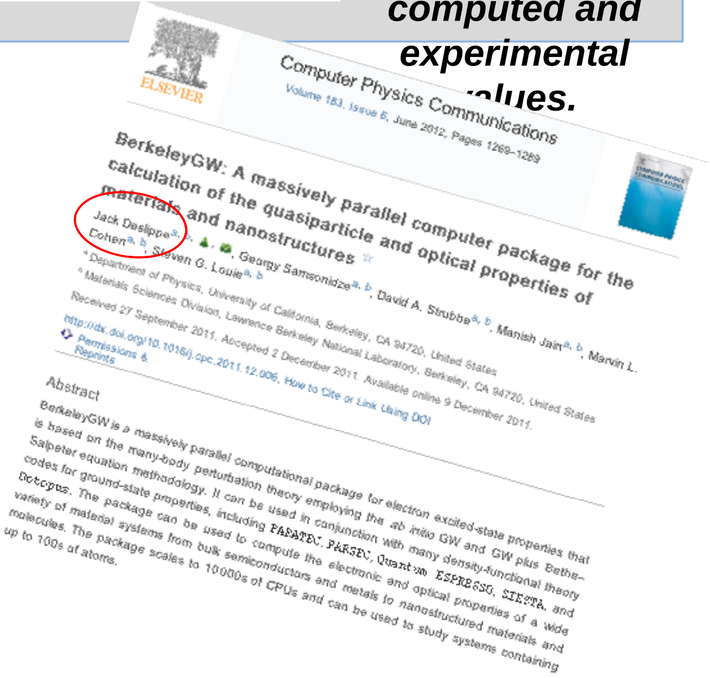
🟢 Bubbles indicate user institutions with size indicating number of users

Important New Method for Studying Solar Materials

- **Goal: develop and use first-principles computational methods to understand, predict, and design novel electronic, optoelectronic, photovoltaic, and thermoelectric materials.**
- **Accomplishment: Using a NERSC NISE award, researchers were able to compute the phonon-assisted interband optical absorption spectrum of silicon entirely from first principles.**
  - **Nearly all commercially-available photovoltaic cells currently depend on this absorption process.**
  - **The new method is general enough to to study fundamental physics of other optoelectronic and photovoltaic materials and can address questions that are not accessible by experiment.**
- **Used the BerkeleyGW software written by new NERSC USG consultant Jack Deslippe.**



Absorption spectrum of silicon for two temperatures showing excellent agreement between computed and experimental values.



Computer Physics Communications

Volume 183, Issue 6, June 2012, Pages 1269–1289

BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures

Jack Deslippe[a, b], Georgy Samsonidze[a, b], David A. Strubbe[a, b], Manish Jain[a, b], Marvin L. Cohen[a, b], Steven G. Louie[a, b]

[a] Department of Physics, University of California, Berkeley, CA 94720, United States

[b] Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States

Received 27 September 2011. Accepted 2 December 2011. Available online 9 December 2011.

http://dx.doi.org/10.1016/j.cpc.2011.12.006, How to Cite or Link Using DOI

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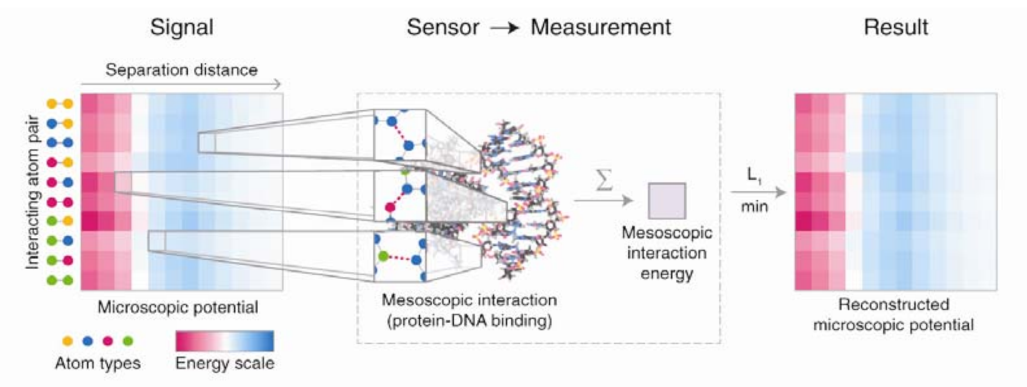
Abstract

BerkeleyGW is a massively parallel computational package for electron excited-state properties that is based on the many-body perturbation theory employing the ab initio GW and GW plus Bethe–Salpeter equation methodology. It can be used in conjunction with many density-functional theory codes for ground-state properties, including PARATEC, PARSEC, Quantum ESPRESSO, SIESTA, and Octopus. The package can be used to compute the electronic and optical properties of a wide variety of material systems from bulk semiconductors and metals to nanostructured materials and molecules. The package scales to 10000s of CPUs and can be used to study systems containing up to 100s of atoms.

PI: E. Kioupakis (U Michigan)

Direct Inference of Protein–DNA Interactions with Compressed Sensing

- "Compressed sensing" determines atomic-level energy potentials with accuracy approaching experimental measurement
  - New technique for finding sparse solutions to underdetermined linear systems
  - "De novo" energy potentials means direct inference — no statistical or physical models
  - Can be applied to other scientific domains, e.g., biofuel production, synthetic biology, materials science
- Using crystal structures and experimental measurements of binding affinity, this method reveals where transcription factors bind with DNA to switch genes on or off
- Will accelerate research in gene expression, gene therapy, etc.



De novo potential determination as an application of compressed sensing. The potential is represented by a heat map of microscopic interaction energies ranging from repulsive (dark pink) to attractive (dark blue). The interatomic protein–DNA potential can be inferred by ℓ1 minimization from measurements provided by a small number of sensors (protein–DNA structures + binding energies).

PI: Harley McAdams, Stanford U.

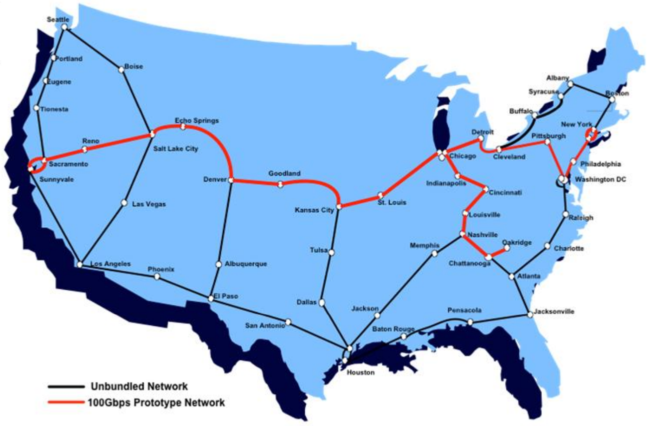
ESnet Upgrade - Ten Times the Bandwidth Over Existing Fiber
Nationwide rollout of 100 gigabit per wavelength service on ESnet

- Sending 10 times more data across existing fiber makes that fiber ten times more valuable.
- Critical bandwidth gain for science but will have impacts across the economy when fully commercialized.

100Gbps Prototype Network

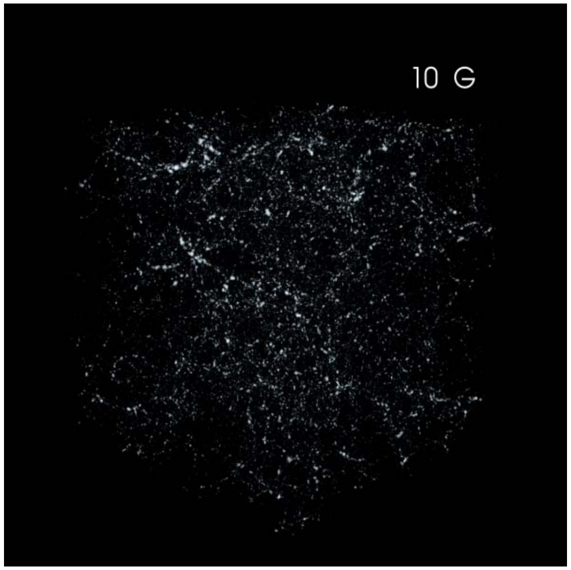
Consists of two elements:

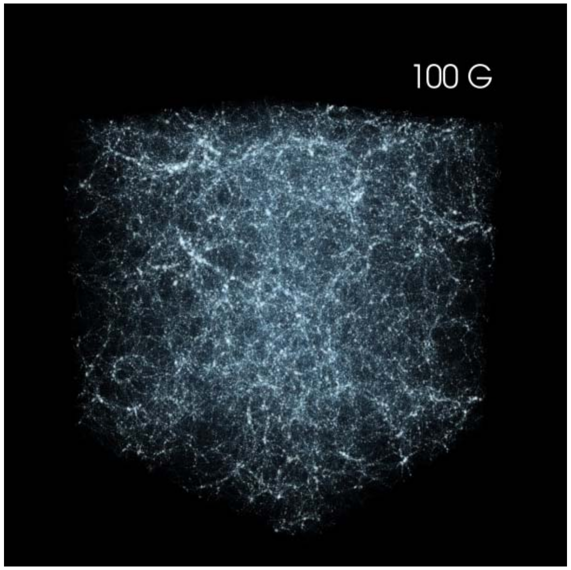
- Backbone network
  - Long haul links between 4 locations
  - Access to 50% of capacity (up to 44 10/40/100Gbps wavelengths)
- Metropolitan networks
  - Last-mile infrastructure to the 4 locations
  - Access to 100% of capacity (up to 88 10/40/100Gbps wavelengths)



Esnet 2012 rolled out map

ESnet Upgrade - Ten Times the Bandwidth Over Existing Fiber
Nationwide rollout of 100 gigabit per wavelength service on ESnet





Model of the early universe. ~13.7 billion years ago, the Universe was near homogenous. Today, the modern Universe is rich in structures that include galaxies, clusters of gravitationally bound galaxies, galaxy super-structures called "walls" that span hundreds of millions of light-years, and the relatively empty spaces between superstructures, called voids.

See the difference 100G can make

Simulation, performed on 4,096 cores of NERSC’s Cray XE6 “Hopper” system produced over 5 terabytes of data that was transferred to the Supercomputing 2011 exhibit floor in Seattle, Washington, in near real-time on ESnet's new 100 gigabit-per-second (Gbps) network. For comparison, a simulation using a 10 Gbps network connection was displayed on a complementary screen to show the difference in quality that an order of magnitude difference in bandwidth can make.

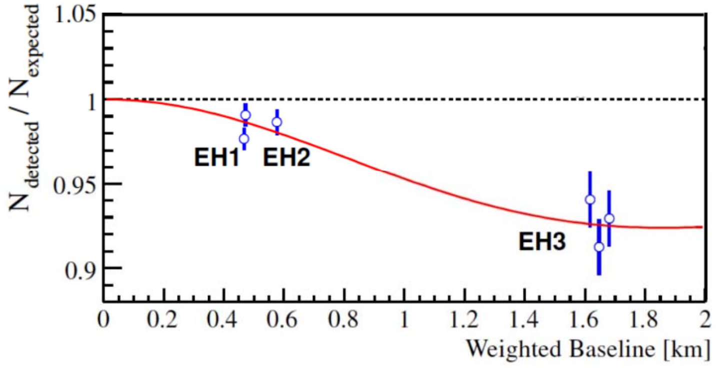
Solving the Puzzle of the Neutrino

- **NERSC and ESnet were vital in the successful measurement of the θ_{13} neutrino transformation.**
  - Last and most elusive piece of a longstanding puzzle: why neutrinos appear to vanish as they travel
  - The answer – a new, surprisingly large type of neutrino oscillation – affords new understanding of fundamental physics; may eventually help solve the riddle of matter-antimatter asymmetry in the universe.

- **Experiment could not have been done without NERSC: PDSF for simulation and analysis; HPSS and data transfer capabilities; and NGF and Science Gateways for distributing results**
  - NERSC is the only site where all raw, simulated, and derived data are analyzed and archived.
  - => Investment in experimental physics requires investment in HPC.

PI: Kam-Biu Luk (LBNL)

HEP



The Daya Bay experiment counts antineutrinos at detectors in three experimental halls (EH) near the Daya Bay nuclear reactor and calculates how many would reach the detectors if there were no oscillation. The plot shows measured disappearance of antineutrinos as a function of distance from the reactor. The 6.0% rate deficit at EH3 provides clear evidence of the new transformation.

NERSC's PDSF cluster

Daya Bay detectors

Research and Evaluation Prototypes

(dollars in thousands)

	FY 2011	FY 2012	**FY 2013**	*Change (FY12 to FY13)*	
Research and Evaluation Prototypes	4,301	30,000	**22,500**	*-7,500*	***-25%***

- *Which computational architectures and platforms will deliver the most benefit for the science of today and the science of the future?*

REP supported development of the Blue Gene architecture – a partnership between IBM, Argonne and Lawrence Livermore national labs . The Blue Gene series was honored with the Medal of Technology and Innovation, October 2009

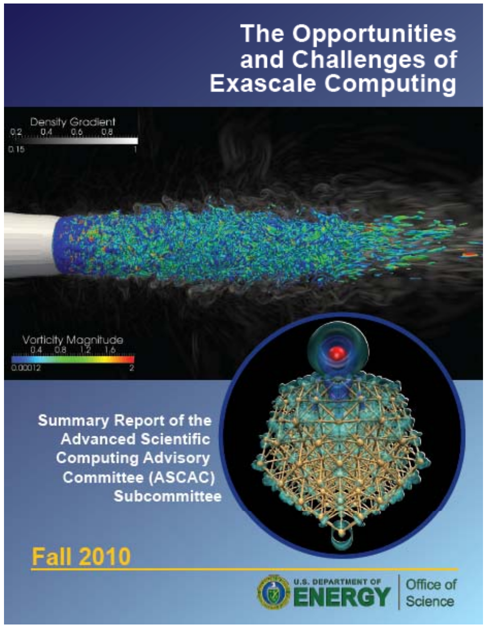
- Addresses the challenges of systems that will be available by the end of the decade
- Prepares researchers to effectively utilize next generation scientific computers
- Reduces the risk of future procurements.
- In FY12, started research partnerships with NNSA to address critical technological issues for exascale computing such as memory, optical networks, etc.
- **In FY13 critical technology partnerships will continue**

ASCR Research

Substantial innovation is needed to provide essential system and application functionality in a timeframe consistent with the anticipated availability of hardware

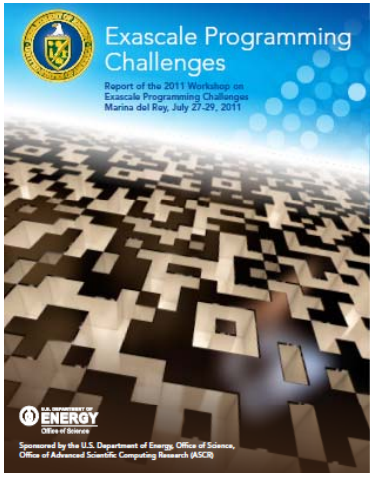
Providing forefront research knowledge and foundational tools since the early 1950's:

- **Applied Mathematics**
- **Computer Science**
- **Computational Partnerships (SciDAC)**
- **Next Generation Networking for Science**


The Opportunities and Challenges of Exascale Computing

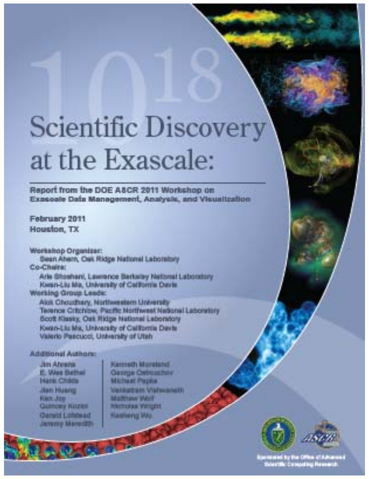
Summary Report of the Advanced Scientific Computing Advisory Committee (ASCAC) Subcommittee

Fall 2010


Exascale Programming Challenges

Report of the 2011 Workshop on Exascale Programming Challenges
Marina del Rey, July 27-29, 2011

Sponsored by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR)


Scientific Discovery at the Exascale:

Report from the DOE ASCR 2011 Workshop on Exascale Data Management, Analysis, and Visualization

February 2011
Houston, TX

Workshop Organizer:
Sean Ahern, Oak Ridge National Laboratory
Co-Chairs:
Arie Shoshani, Lawrence Berkeley National Laboratory
Kwan-Liu Ma, University of California Davis
Working Group Leads:
Alok Choudhary, Northwestern University
Terence Critchlow, Pacific Northwest National Laboratory
Scott Klasky, Oak Ridge National Laboratory
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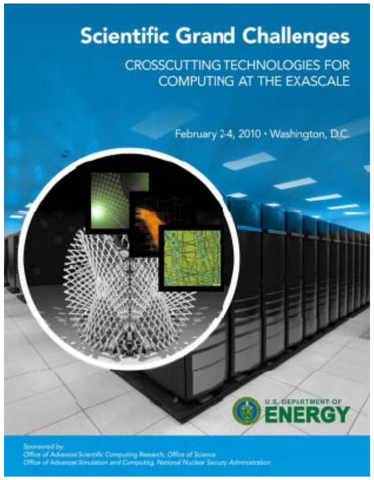

Scientific Grand Challenges

CROSSCUTTING TECHNOLOGIES FOR COMPUTING AT THE EXASCALE

February 2-4, 2010 • Washington, D.C.

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

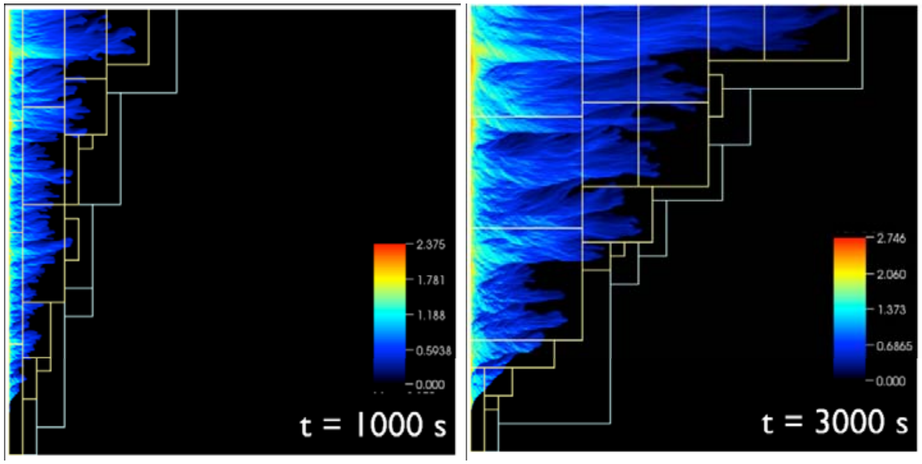
RAPTOR NETWORKS TECHNOLOGY INC
absoft
SMC Networks
IBM
intel
Linux
ROGUE WAVE SOFTWARE
amazon webservices
extreme networks
MathWorks
ADVA Optical Networking
INTERNET2
NVIDIA
NETEFFECT
hp
YAHOO!
NETGEAR
CISCO
ciena
JUNIPER NETWORKS
DELL
FORCE10
CRAY
QLOGIC
Myricom
Microsoft
BROCADE
python
Alcatel·Lucent
AMD

Applied Mathematics

(dollars in thousands)

	FY 2011	FY 2012	**FY 2013**	*Change (FY12 to FY13)*	
Applied Mathematics	45,604	45,604	**49,500**	*+3,896*	***+8.5%***

- *What new mathematics are required to accurately model complex systems such as plasma containment in a Tokamak or the electric power grid taking place on vastly different time and/or length scales?*



Extended AMR capability for subsurface modeling of multicomponent, multiphase compressible flows - now being used by EM as part of the ASCEM project

- **Mathematics for Data-intensive Science (increased in FY13)**
- Uncertainty Quantification (Increased in FY12)
- Numerical methods
- Advanced linear algebra
- Computational meshing
- Optimization algorithms
- Multiscale mathematics and multiphysics
- Joint Applied Mathematics-Computer Science Institutes
- Mathematics of cyber security basic research
- Computational Science Graduate Fellowship

DOE Computational Science Graduate Fellowship (DOE CSGF)

- Started in 1991 because of the critical importance of computational science to the Nation and DOE's need for **broadly trained** advanced computational scientists
- Funded by both DOE-SC/ASCR and NNSA/ASC
- Requires that fellows
  - plan and follow a plan of study that transcends the bounds of traditional academic disciplines
  - participate in 12-week research experience at DOE lab
- Benefits
  - Up to four years of support subject to renewal each year
  - Full tuition and required fees will be paid during the appointment period
  - Yearly stipend of $36,000
  - Academic allowance of $5,000 the first year and $1,000 in the remaining years for the professional development of the fellow
- CSGF Alumni:
  - Working at DOE labs, companies (IBM, GE, P&G, Intel, Pratt &Whitney, etc),universities (Duke, Stanford, UC, etc.)
- 2012-13 academic year: 729 applicants for 21 awards

The Subcommittee believes that the CSGF is unique in its focus on Computational Science. It provides features that other Graduate research Fellowships do not, such as the Plan of Study, the Practicum, the Annual CSGF Conference and efforts to keep alumni engaged. In this regard, the CSGF is an exceptional program that produces interdisciplinary scientists uniquely qualified to address current and future computational science challenges.

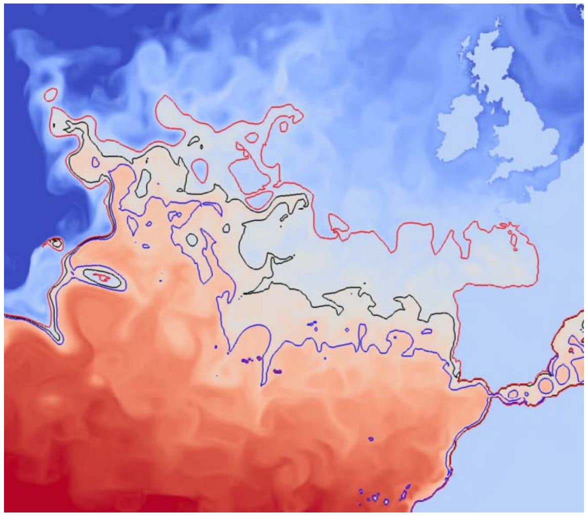
2011 ASCAC Review of DOE Computational Science Graduate Fellowship Program

Computer Science

(dollars in thousands)

	FY 2011	FY 2012	**FY 2013**	*Change (FY12 to FY13)*	
Computer Science	47,301	47,400	**54,580**	*+7,180*	***+15%***

- *What operating systems, data management, analysis, representation model development, user interface, and other tools are required to make effective use of current and future-generation supercomputers?*



Quantified data reduction reduces time to visual understanding of remote data. Technique available in widely used open-source visualization tool and toolkit

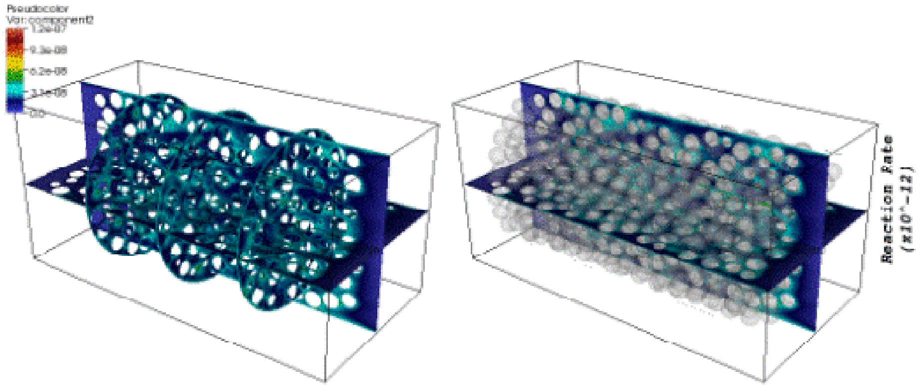
- **Computer Science research for Data-intensive Science (New in FY13 building on core investments in data focused on needs of SC programs)**
- Extreme Scale Operating and file systems.
- Performance and productivity tools
- Programming models
- Data management and visualization
- Joint Applied Mathematics-Computer Science Institutes
- Pre-competitive research in advanced computer architectures

Computational Partnerships (SciDAC)

(dollars in thousands)

	FY 2011	FY 2012	**FY 2013**	*Change (FY12 to FY13)*	
Computational Partnerships	52,813	44,250	**56,776**	*+12,526*	***+28%***

- *What advances in computer science and mathematics could enable researchers to more accurately model systems such as the earth's climate, bioenergy, nano-materials and other areas important to DOE missions?*

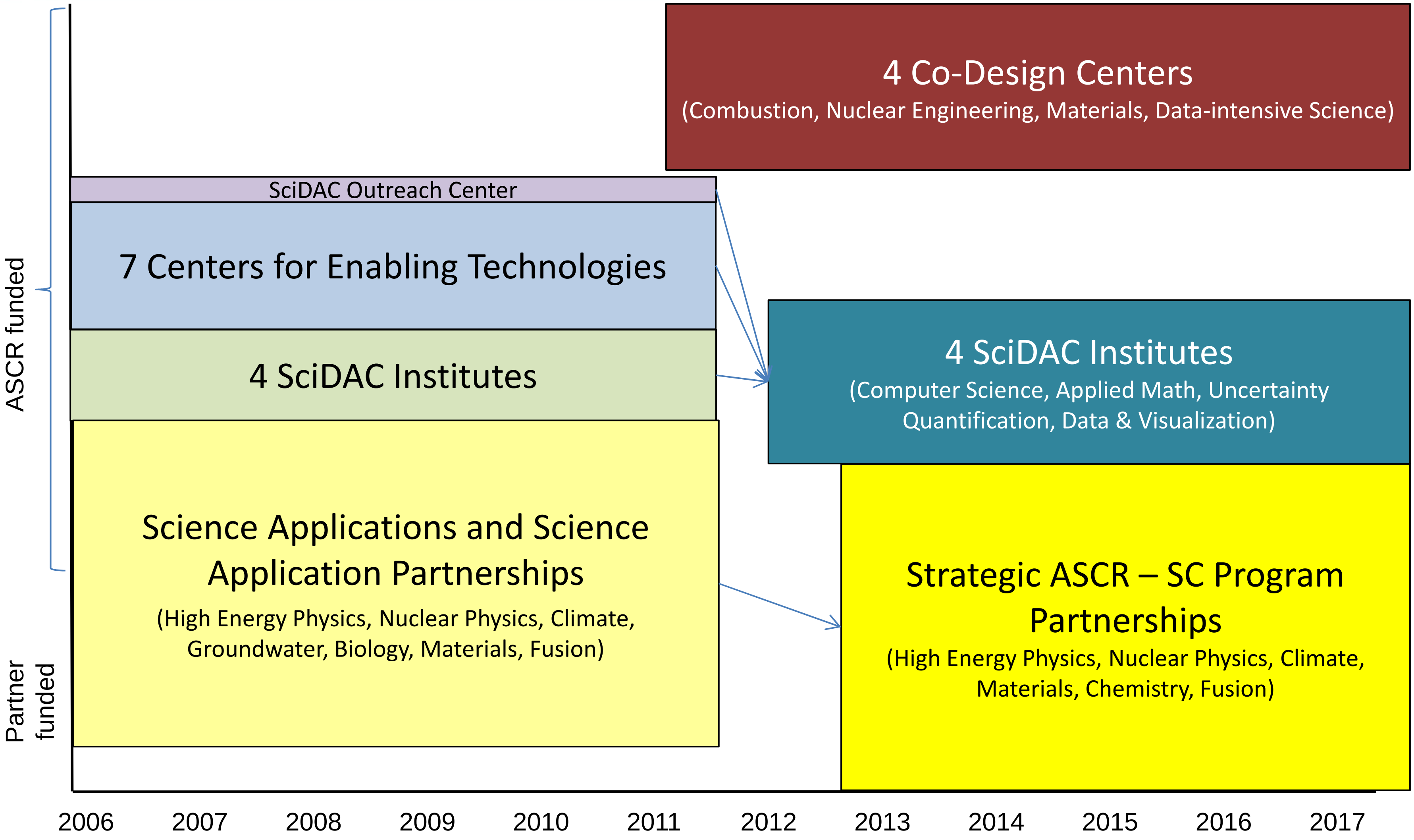


SciDAC-e visualization and analysis tools provide new ways for developing technology to store CO2 safely in deep surface rock formations to reduce the amount of CO2 in the atmosphere

SciDAC recompeted in FY12

- SciDAC Institutes
  - Four new SciDAC Institutes replace the 12 Centers and Institutes from SciDAC 2
  - Provides more effective support to applications
- Strategic ASCR-SC Program Partnerships
  - Enabling strategic advances in program missions
  - **New FY13 partnerships will focus on specific data issues of partner facilities/collaborations**
- Co-Design Centers
  - Close coupling of applications, computer science, and computer hardware architecture that is required for success at exascale.
  - **New in FY13 Data-intensive Science Co-design**

SciDAC Portfolio Timeline



Strategic ASCR – SC Program Partnerships

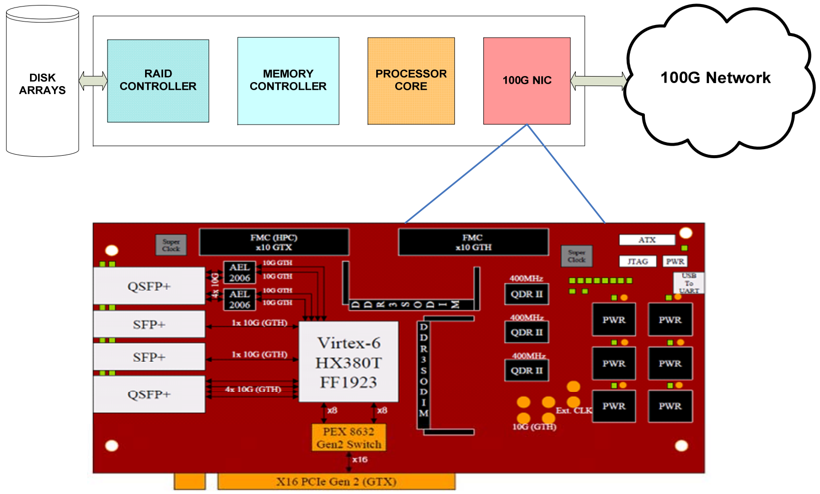
- **Goals and Objectives**
  - Partner with SC Programs to combine the best applied mathematics, computer science, and networking with SC program expertise to enable Strategic advances in program missions.
- **Five FOAs – Proposals out for joint review:**
  - Fusion Energy Science: topics in Edge Plasma Physics, Multiscale Integrated Modeling, and Materials Science
  - High Energy Physics: topics in Cosmological Frontier, Lattice Gauge Theory QCD, and Accelerator Modeling and Simulation
  - Nuclear Physics: topics in Low- and Medium-Energy Nuclear Physics and Heavy Ion Collider Physics
  - Biological and Environmental Research: topics in dynamics of atmospheres, oceans, and ice sheets that support Earth System Modeling
  - Basic Energy Sciences: topics in theoretical chemistry and materials science, especially excited states of atoms and molecules, materials electron correlation.

Next Generation Networking for Science

(dollars in thousands)

	FY 2011	FY 2012	**FY 2013**	*Change (FY12 to FY13)*	
Next Generation Networking for Science	12,313	12,751	**16,194**	*+3,443*	***+27%***

- *What tools are needed to make all scientific resources readily available to scientists, regardless of whether they are at a national laboratory, university, or industrial setting?*



End-system network interface controller for 100Gbps wide area networks extends 100G capability for full end-to-end connectivity. Accelerates transfer of massive data sets between DOE labs and research institutions.

- **Distributed Data-intensive Science (increased in FY13)**
- Distributed systems software including scalable and secure tools and services to facilitate large-scale national and international scientific collaborations.
- Advanced network technologies including dynamic optical network services, scalable cyber security technologies, and multi-domain, multi-architecture performance protocols to seamlessly interconnect and provide access to distributed computing resources and science facilities.

Workshops

- Dec 6-7, 2011 Scientific Collaborations for Extreme Scale Science Workshop
  Gaithersburg Marriott Washingtonian Center, Gaithersburg, MD; report at
  http://science.energy.gov/~/media/ascr/pdf/program -documents/docs/Scientific_Collaborations_for_Extreme_Scale_Science_Report_Dec_2011_Final.pdf
- January 17, 2012 Exascale Summit
  American Geophysical Union, Washington, DC
- February 21-24, 2012 Resiliency Workshop
  Catonsville, MD
- March 6, 2012 Modeling of Exascale Applications on Exascale Systems Summit
  American Geophysical Union, Washington, DC
- March 7, 2012 DOE Applied Math Summit
  American Geophysical Union, Washington, DC
- March 8-9, 2012 Extreme Scale Solvers Workshop
  American Geophysical Union, Washington, DC
- March 19-20, 2012 Computing Electrical and Optical Technologies for Computing Interconnectivity Workshop
  American Geophysical Union, Washington, DC
- March 29-30, 2012 Applied Math Principle Investigators Meeting
  American Geophysical Union, Washington, DC
- April 16-20, 2012 Exascale Research Principle Investigators Meeting
  University of Oregon, Portland, OR
- May, 2012 Resilience Workshop
  TBD, DC area
- May 8-9, 2012 Transforming Geant4 for the Future
  Rockville Hilton, Rockville, MD
- June, 2012 Fault Management Workshop
  TBD, DC area
- July, 2012 Data Intensive Science Workshop
  TBD, DC area
- September 11-12, 2012 Exploratory Workshop
  American Geophysical Union, Washington, DC

ASCR at a Glance

Office of Advanced Scientific Computing Research

Associate Director – Daniel Hitchcock
Phone: 301-903-7486
E-mail: Daniel.Hitchcock@science.doe.gov

Research

Division Director – William Harrod
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E-mail: William.Harrod@science.doe.gov

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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

Three Exascale Co-Design Centers Awarded

Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)

Director: Timothy Germann (LANL)

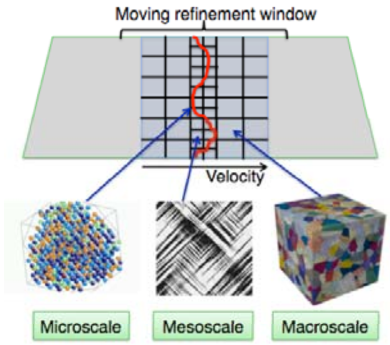
Center for Exascale Simulation of Advanced Reactors (CESAR)

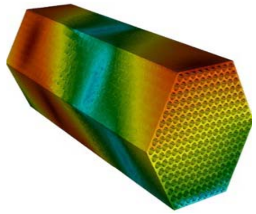
Director: Robert Rosner (ANL)

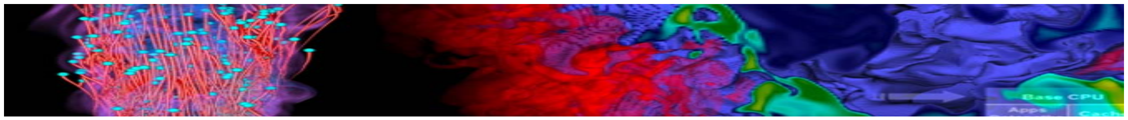
Combustion Exascale Co-Design Center (CECDC)

Director: Jacqueline Chen (SNL)

	ExMatEx (Germann)	CESAR (Rosner)	CECDC (Chen)
National Labs	LANL	ANL	SNL
	LLNL	PNNL	LBNL
	SNL	LANL	LANL
	ORNL	ORNL	ORNL
		LLNL	LLNL
			NREL
University & Industry Partners	Stanford	Studsvik	Stanford
	CalTech	TAMU	GA Tech
		Rice	Rutgers
		U Chicago	UT Austin
		IBM	Utah
		TerraPower	
		General Atomic	
		Areva	







The four SciDAC Institutes are large team projects involving National Lab, University and Industry collaborators

FASTMath **Director – Lori Diachin, LLNL**	**QUEST** **Director – Habib Najm, SNL**	**SUPER** **Director – Robert Lucas, USC**
Lawrence Livermore (CA)	**Sandia (NM)**	**University of Southern CA**
Argonne (IL)	Los Alamos (NM)	Argonne (IL)
Lawrence Berkeley (CA)	Johns Hopkins University (MD)	Lawrence Berkeley (CA)
Sandia (CA and NM)	Massachusetts Institute for Technology (MIT – MA)	Lawrence Livermore (CA)
Rensselaer Polytechnic Institute (NY)	University of Southern California (CA)	Oak Ridge (TN)
	University of Texas at Austin (TX)	University of CA, San Diego (CA)
		University of Maryland (MD)
		University of North Carolina (NC)
		University of Oregon (OR)
		University of Tennessee, Knoxville (TN)
		University of Utah (UT)

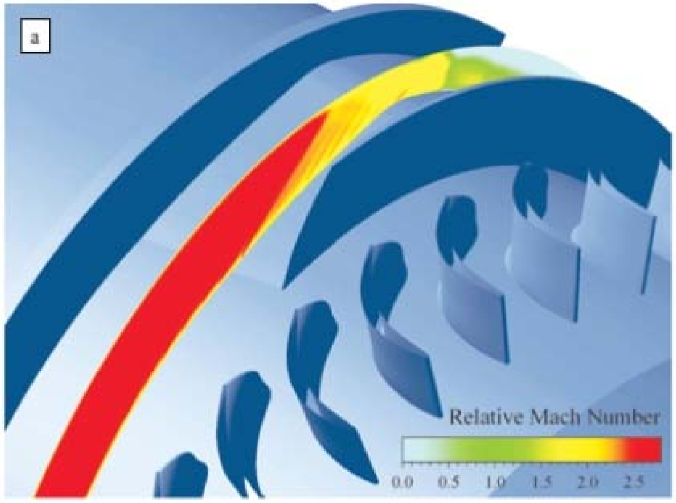
🟨 **Lead**
🟩 Labs
🟦 Universities

The SciDAC Institute for Data and Visualization will be announced in late March 2012

Example: New Turbo Compressors Reduce the Cost of Carbon Capture and Sequestration

OLCF helped Ramgen go from computer design to cutting Titanium in two months

- **CO_2 compressors are a large fraction of the cost of Carbon Capture and Sequestration (CCS)**
- **Ramgen Power Systems is developing shock compression turbo machinery to reduce CCS costs**
  - A complementary goal for Ramgen's innovations is lower cost, more efficient gas turbines for electricity generation
- **Ramgen has significantly advanced its shock wave based compression aerodynamic design process**
  - Observed designs that exhibit valuable new characteristics, only possible with OLCF's Jaguar supercomputer
- **A new workflow paradigm shortens a more comprehensive design cycle for the compressors**



Computational Fluid Dynamics model of Rampressor-2 inlet guide vane row and rotor

"Ramgen Power Systems would like to thank the Oak Ridge Leadership Computing Facility for helping us utilize Jaguar to the fullest potential, and drive innovations in a technology that will result in highly important products for the United States and the world."

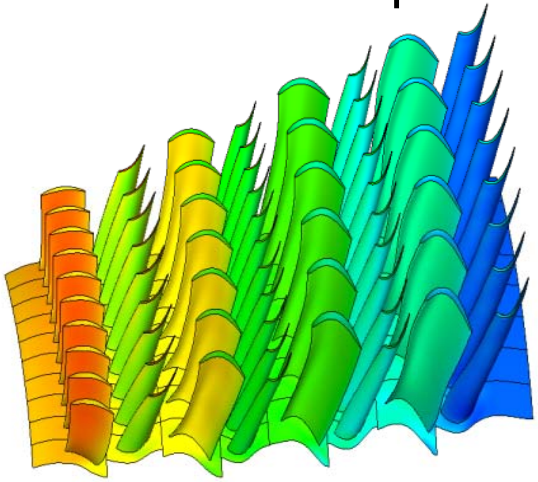
- Allan Grosvenor, Ramgen Power Systems

RAMGEN POWER SYSTEMS™

Example: Design of Fuel Efficient, Low Noise Jet Engines

Results provided substantial ROI justification for GE to purchase its own supercomputer

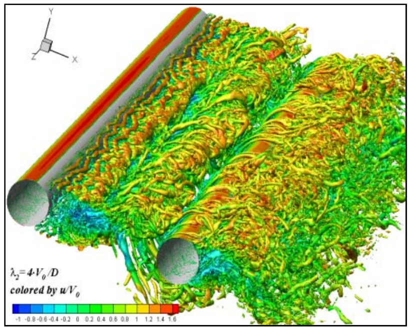
- **General Electric ran their largest-ever CFD calculation to advance study of turbomachinery**
- **Studied for the first time unsteady flow characteristics in turbomachinery. This permitted comparative study of traditional turbine CFD analysis (steady flow) vs. unsteady flow analysis with and without mid-frame strut for a low pressure turbine**
- **Simulations evolved from 3-D to 4-D**
- **Identified efficiency shifts in each stage**
- **Discovered new insight into the behavior of secondary flows: vortical, high entropy flows near the hub and casing**



Simulation domain: 8 blade rows, first four stages of a 7-stage low pressure turbine: 200M grid cells, 180K iterations

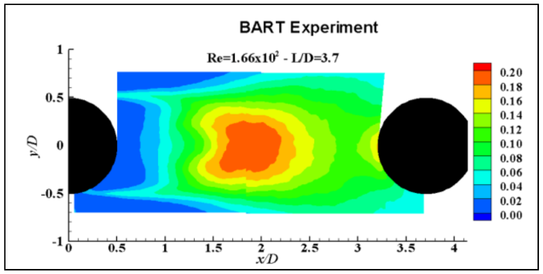
Example: Quieter Planes

Landing gear of Boeing 777

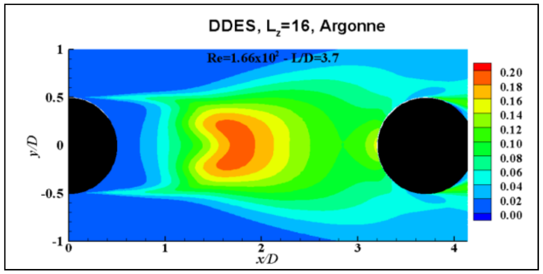


Tandem cylinder used for V&V

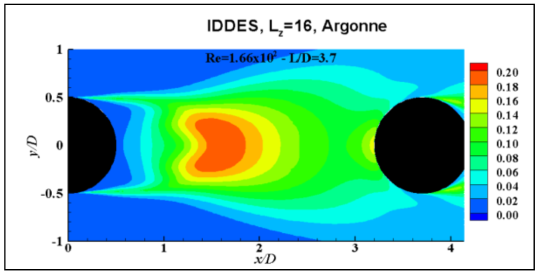
- **Boeing is using ALCF to simulate turbulence created by aircraft landing gear and to calculate the noise caused by two cylinders placed in tandem in an air stream.**
- **Boeing expects these capabilities to contribute to the design of safe and quiet technologies**
- **The simulations are being carried out on eight 192 nodes (i.e. 32,768 cores) of the Blue Gene/P. The code used is the multi-purpose CFD code NTS. It allows Delayed Detached-Eddy Simulation(DDES) and Improved Delayed Detached-Eddy Simulations (IDDES) to be compared, to each other and to experimental data.**



Experiment used as baseline



DDES method run at ALCF



IDDES method run at ALCF