View from Washington

August 23, 2011

ASCAC

Daniel Hitchcock

Acting Associate Director

Advanced Scientific Computing Research

Advanced Scientific Computing Research

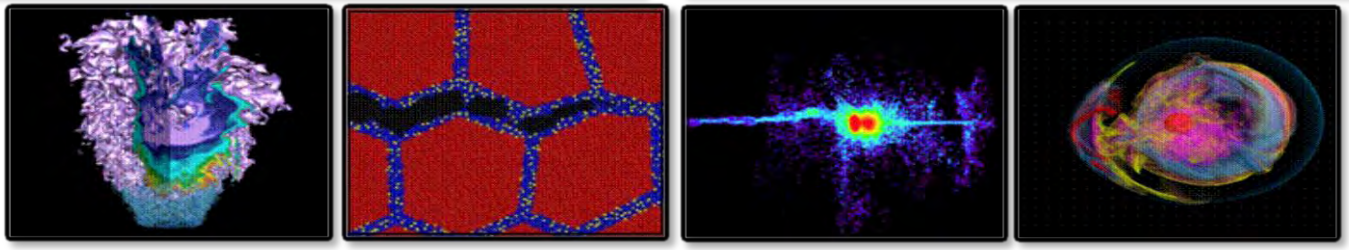
Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

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

(dollars in thousands)

	FY 2011 Budget	FY 2012 Request	FY 2012 House	FY 2012 vs. FY 2011	FY 2012 vs. House
Advanced Scientific Computing Research					
Exascale — Applied Mathematics	45,450	48,973		+ 3,523	
Exascale — Computer Science	47,400	47,400		–	
Exascale — Computational Partnerships (includes SciDAC)	53,297	60,036		+ 6,739	
Next Generation Networking for Science	14,195	12,751		-1,444	
SBIR/STTR	4,619	4,873		+ 254	
Total, Mathematical, Computational, and Computer Sciences Research	*164,961*	*174,033*		*+9,072*	
High Performance Production Computing (NERSC)	56,000	57,800		+ 1,800	
Leadership Computing Facilities	158,000	156,000		- 2,000	
Exascale — Research and Evaluation Prototypes	5,980	35,803		+29,923	
High Performance Network Facilities and Testbeds (ESnet)	30,000	34,500		+ 4,500	
SBIR/STTR	7,056	7,464		+ 408	
Total, High Performance Computing and Network Facilities	*257,036*	*291,567*		*+34,531*	
Total, Advanced Scientific Computing Research	**421,997**	**465,600**	**427,093**	**+ 43,603**	**- 38,507**

ASCR FY12House Budget Language

- ADVANCED SCIENTIFIC COMPUTING RESEARCH

  The Advanced Scientific Computing Research program develops world-leading computing and networking capabilities in support of science and energy research. The Committee recommends $427,093,000 for Advanced Scientific Computing Research, $5,096,000 above fiscal year 2011 and $38,507,000 below the request.

  The Office of Science and the National Nuclear Security Administration fund the development and operation of the world's fastest computing systems. These systems have consistently topped the list of the world's fastest supercomputers. More than just symbolic, American leadership in supercomputing supports domestic world leading weapons and scientific research while keeping the private sector at the leading edge of information technology. Global competition has become increasingly fierce, with the United States unseated from the top spot in late 2010. The Committee continues to support science activities in the United States that improve and develop the world's fastest supercomputing systems.

ASCR FY12House Budget Language

- ADVANCED SCIENTIFIC COMPUTING RESEARCH (cont.)

  Exascale Computing.—Beyond short-term incremental improvements in leadership computing systems, the Department is currently conducting research into the development of an exaflop speed—or ''exascale''—computing platform that would run at three orders of magnitude faster than today's fastest computing systems. The pursuit of computing capabilities at these speeds is crucial to maintaining U.S. leadership in the increasingly important field of high performance computing, and in the broader information technology industry. Further, exascale systems will enable new simulations and analyses not currently possible in basic science research, energy technology development and weapons science. As both the Office of Science and the National Nuclear Security Administration have vested interests in exascale computing, the Committee commends efforts to collaborate on exascale research across these two programs and encourages further coordination and collaboration.

ASCR FY12House Budget Language

- ADVANCED SCIENTIFIC COMPUTING RESEARCH (cont.)

  While the budget request proposes funding increases to accelerate exascale research and emphasizes its importance, the Department has not yet aggregated exascale research components into a coherent effort. Several Department national laboratories have stated target years for exascale prototypes and fully-operational exascale systems, but the Department has not stated any such timeframes, nor has it provided clear funding amounts for the exascale effort in the budget request. The Department is directed to provide to the Committee, not later than February 10, 2012, a report including its current target date for developing an operational exascale platform, interim milestones towards reaching that target, estimated total ranges of Department investment likely needed to hit those targets, and a complete listing of exascale activities included in the budget request broken out by program and activity with comparisons to the current year's funding levels.

See Bill Harrod's talk on ASCR's Exascale effort tomorrow at 8:30

ASCR FY12House Budget Language

- ADVANCED SCIENTIFIC COMPUTING RESEARCH (cont.)

  The Committee is supportive of investment in the national laboratories to expedite the exascale initiative, but also recognizes that small technology companies frequently provide the breakthrough innovations that are needed to achieve the kind of low power, high-speed systems needed for exascale computing, particularly as the leap to exascale may require unconventional technology solutions. For this reason, the Committee encourages the Department not to limit its exascale efforts solely to national laboratories and the largest private sector organizations, but also to consider small companies and research organizations working on the cutting edge of computing technologies.

See Walt Polansky's talk on ASCR's new approach to SBIR tomorrow at 11:45

Looking Backward and Forward

SciDAC Centers for Enabling Technology and Institutes

Science Application Partnerships

Hopper
Jaguar
Intrepid

Many Core Energy Aware

X Stack

CoDesign

SciDAC Institutes

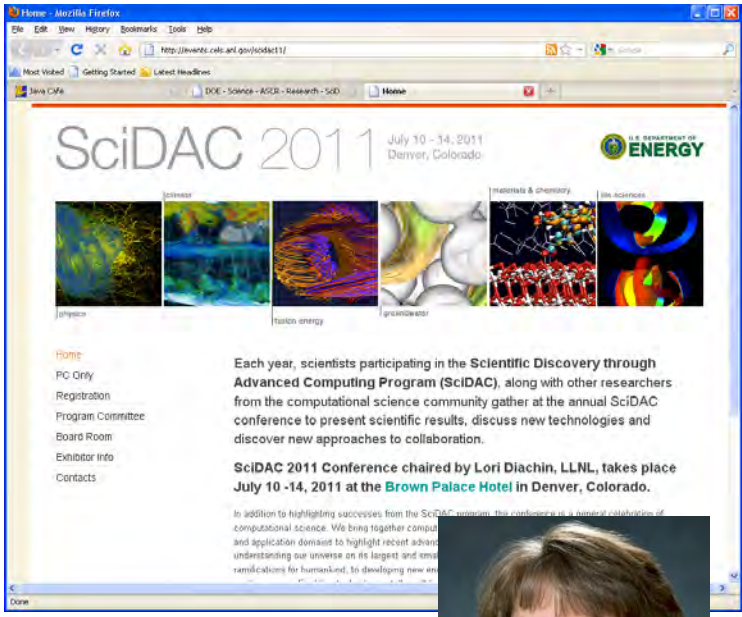
Strategic ASCR – SC Office Partnerships

Titan
Mira
???

SciDAC 2011 Conference

"Addressing the Challenges of the Next Decade"

- 377 participants from a broad range of computational science areas expected
- Special Activities:
  - Poster sessions including early career/CSGF
  - Viz Night
    - Information Presentation Winner:
      - Shock Wave/turbulence boundary interaction - M. Matheson, *et al*
    - Visual Aesthetics winner:
      - Magnetic Field Outflows from Active Galactic Nuclei - D. Pugmire, *et al*
- Special thanks to:
  - Lori Diachin and the Technical Program Committee
  - Argonne National Laboratory Staff
  - Vendor Supporters



Conference Chair:
Lori Diachin, LLNL

SciDAC
Scientific Discovery through Advanced Computing

Presentation materials available at http://events.cels.anl.gov/scidac11/agenda-2/

Recent DOE Funding Opportunity: Scientific Discovery through Advanced Computing (SciDAC) Institutes

Program Funding – DOE, Office of Advanced Scientific Computing Research (ASCR)

- Up to $13M/year for 5 years may be available to support between 1 and 5 SciDAC Institutes
- DOE National Laboratories, Universities, Industry and other organizations may apply
- "The overall portfolio and management of Institute awards is expected to cover a significant portion of DOE computational science needs on current and emerging computational systems."

Specific goals and objectives for SciDAC Institutes

- Tools and resources for lowering the barriers to effectively use state-of-the-art computational systems;
- Mechanisms for taking on computational grand challenges across different science application areas;
- Mechanisms for incorporating and demonstrating the value of basic research results from Applied Mathematics and Computer Science; and
- Plans for building up and engaging our nation's computational science research communities.

Timeline

- Issued - **February 23, 2011**
- LOI, not required, - **March 30, 2011**
- Application due date – **May 2, 2011**
- FY11 awards – **July 2011**

Budget summary:

37 Institutes - Letters of Intent requesting $217M/year

27 Institutes - Full proposals requesting $141M/year

20 Institutes reviewed at total of $106M/year

3 Institutes awarded at total of $10.5M/year

Scientific Discovery through Advanced Computing (SciDAC) Institutes – FY11 Awards

FASTMath – Frameworks, Algorithms, and Scalable Technologies for Mathematics

Topic areas: Structured & unstructured mesh tools, linear & nonlinear solvers, eigensolvers, particle methods, time integration, differential variational inequalities

QUEST – Quantification of Uncertainty in Extreme Scale Computations

Topic areas: Forward uncertainty propagation, reduced stochastic representations, inverse problems, experimental design & model validation, fault tolerance

SUPER – Institute for Sustained Performance, Energy and Resilience

Topic areas: Performance engineering (including modeling & auto-tuning), energy efficiency, resilience & optimization

FASTMath Director – Lori Diachin, LLNL	QUEST Director – Habib N. Najm, SNL	SUPER Director – Robert F. Lucas, USC
Argonne National Laboratory	Los Alamos National Laboratory	Argonne National Laboratory
Lawrence Berkeley National Lab	**Sandia National Laboratories***	Lawrence Berkeley National Lab
Lawrence Livermore National Lab*	Johns Hopkins University	Lawrence Livermore National Lab
Sandia National Laboratories	Massachusetts Institute of Technology	Oak Ridge National Laboratory
Rensselaer Polytechnic Institute	University of Southern California	University of California at San Diego
	University of Texas at Austin	University of Maryland
		University of North Carolina
		University of Oregon
		University of Southern California*
		University of Tennessee at Knoxville
		University of Utah

New DOE Funding Opportunities: SC Application Partnerships with SciDAC Institutes

DOE Office of Science is lead federal agency in fundamental research for energy

- SC is comprised of 6 interdisciplinary scientific program offices
- Nation's largest supporter of basic research in the physical sciences
- Unique open-access scientific user facilities – including leadership-class supercomputers

Overview of funding opportunities for Application Partnerships

- Each FOA issued by an SC office & in partnership with ASCR
- DOE National Laboratories, Universities, Industry and other organizations may apply
- Partnerships will exploit leadership-class computing resources to advance scientific frontiers in areas of strategic importance to the Office of Science
- Partnerships will effectively leverage the SciDAC Institutes' intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools

Timeline for Partnerships FOAs

- SC Application Partnerships in Fusion Energy Science: DE-FOA-0000571, LAB 11-571
  - ✓ Posted August 3; Pre-proposals due September 9; Proposals due October 26
- FOAs are also being developed in partnership with other SC offices
- First awards expected in mid-FY12

Strategic ASCR – SC Office Partnerships

Goals & Objectives

- Partner with SC Programs to Combine the best math, CS, and networking with SC program expertise to enable *strategic* advances in program missions

Eligible applicants- DOE National Laboratories, Universities, Industry and other organizations

Expected outcome- New Science.

Awards Timeline – Joint FOA's in development with other SC Offices

- Solicitations open:
  - Scientific Discovery through Advanced Computing: Scientific Computation Application Partnerships in Fusion Energy Science
    - Issued August 3, 2011
    - Preapplications are required and must be submitted by September 9, 2011
    - Application Due Date: October 26, 2011, 11:59 PM Eastern Time
- Anticipate Solicitations soon in Climate, Nuclear Physics, and High Energy Physics
- Anticipate Awards- mid FY2012

Co-Design

Goals & Objectives

- **Understand how to allocate complexity between hardware, systems software, libraries, and applications;**
- **Modify application designs at all levels;**
- **Understand reformulating as well as reimplementing tradeoffs;**
- **Explore uncertainty quantification, in line data analysis, and resilience in applications;**
- **Co-adapt applications to new programming models and perhaps languages;**
- **Impact of massive multithreaded nodes and new ultra-lightweight operating systems.**

Awards- June 2011

Expected outcome- Understanding, Guidance for Future Applications, Application Readiness

See Timothy Germann's talk on the ExMatEx Co-design Center today at 10:50

Three Exascale Co-Design Centers Awarded

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

Director: Timothy Germann (LANL)

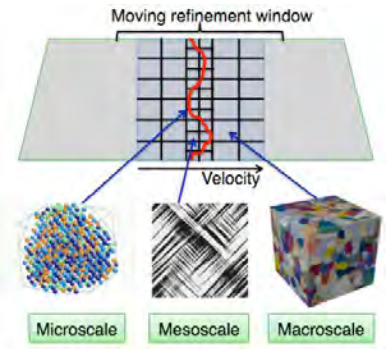
Center for Exascale Simulation of Advanced Reactors (CESAR)

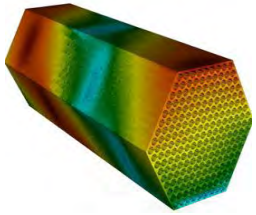
Director: Robert Rosner (ANL)

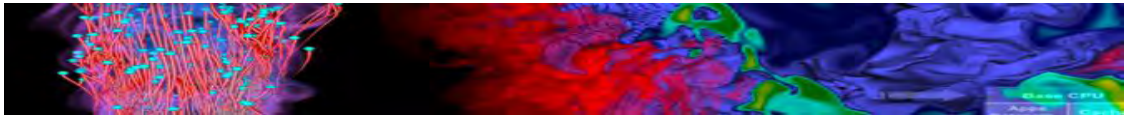
Combustion Exascale Co-Design Center (CECDC)

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	





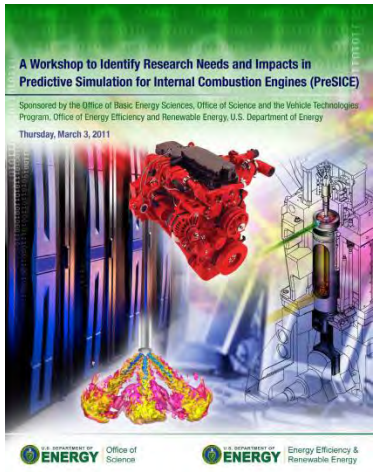


ASCR Interactions with Applied Programs

- **BES/EERE Workshop - Predictive Simulation for Internal Combustion Engines (PreSICE) -March 3, 2011**

  Finding: "Current understanding and modeling capability of stochastic processes in engines remains limited and prevents designers from achieving significantly higher fuel economy."

  Final Report:
  http://www1.eere.energy.gov/vehiclesandfuels/pdfs/presice_rpt.pdf



- **Office of Electricity Delivery and Energy Reliability (OE) Workshop: *Computational Needs for the Next Generation Electric Grid* April 18-20, 2011, Cornell University**
  - Purpose: bring together experts from various fields of computation to discuss current industry practice and provide a critical comparative review of relevant research during the next 5 to 10 years.
  - Outcome: Final report pending; increased interactions between SC, OE, ARPA-E, and EERE on modeling and simulation of "complex systems of systems"

The contiguous U.S. electric power transmission grid. New computational modeling and analysis tools are needed that integrate real-time information to optimize power flow and prevent outages.

See Michael McQuade's talk on Design & Control of Dynamic Energy Systems at 3:15
And Chris Hart's talk on Fundamental problems of Wind energy and HPC

Future of Data Driven Science

- **All of these hardware trends impact data driven science (in many cases more than compute intensive);**
- **Data from instruments still on 18-24 month doubling because detectors on CMOS feature size path;**
- **100 gigabit per second per lambda networks on horizon;**
- **Disk read and write rates will fall further behind processors and memory;**
- **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 users laptop is not friendly)**

See Mario Campolargo's talk on EU Data Initiative today at 1:45

ASCR-BES Workshop on Data

"Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery"

October 24-25, 2011 **Bethesda, MD**

Goals & Objectives

- **Identify and review the status, successes, and shortcomings of current data (including analysis and visualization) and communication pathways for scientific discovery in the basic energy sciences;**
- **Ascertain the knowledge, methods and tools needed to mitigate present and projected data and communication shortcomings;**
- **Consider opportunities and challenges related to data and communications with the combination of techniques (with different data streams) in single experiments;**
- **Identify research areas in data and communications needed to underpin advances in the basic energy sciences in the next ten years;**
- **Create the foundation for information exchanges and collaborations among ASCR and BES supported researchers, BES scientific user facilities and ASCR computing and networking facilities.**

Co-Chairs

- **Peter Nugent, NERSC**
- **J. Michael Simonson, SNS**

Research Progress

- **July 27-29, 2011 Programming Challenges Workshop**
  - USC/ISI, Marina del Rey, CA
- **August 2-3, 2011 2011 Workshop on Architectures I: Exascale and Beyond: Gaps in Research, Gaps in our Thinking**
  - Stanford, CA
- **August 8-10, 2011 2011 Workshop on Architectures II: Exascale and Beyond: Configuring, Reasoning, Scaling**
  - Sandia National Laboratories, Albuquerque, NM
- **August 8-10, 2011 HEC File Systems and I/O (FSIO) Conference**
  - Arlington, VA
- **August 16-19, 2011 12th Workshop on the DOE Advanced CompuTational Software (ACTS) Collection**
  - Lawrence Berkeley National Laboratory, Berkeley, CA
- **October 6-7, 2011 4th Extremely Large Databases (XLDB4) Conference**
  - Menlo Park, California
- **October 11-13, 2011 Exascale Research Principal Investigators Meeting**
  - Washington, DC
- **October 17-19, 2011 Applied Mathematics Principal Investigators Meeting**
  - Hyatt Regency Reston, Reston, VA
- **October 18-19, 2011 GRDI2020: "Global Research Data Infrastructures: The Big Data Challenges"**
  - Brussels, Belgium
- **October 23-14, 2011 IEEE VisWeek 2011**
  - Providence, RI

Back to the Future

- **Math Ideas from 70's that may be relevant for manycore:**
  - More complex basis functions---All those Bessel functions, Hypergeometric functions etc can be computed thru recursion.
- **Coordinate transformations--- Can you deform space so you can use a uniform mesh?**
- **Method of averaging to deal with stiffness---**
  - Only need time averages on fast time scale;
  - Local time averages can be done without leaving chip (maybe)
  - Trades flops for memory access
  - Works for strong mixing stochastic systems too
- **Role of stochastic systems in solving problems---**
  - Positive Lyapunov numbers amplify noise
  - Uncertainty quantification/What are you allowed to measure.

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

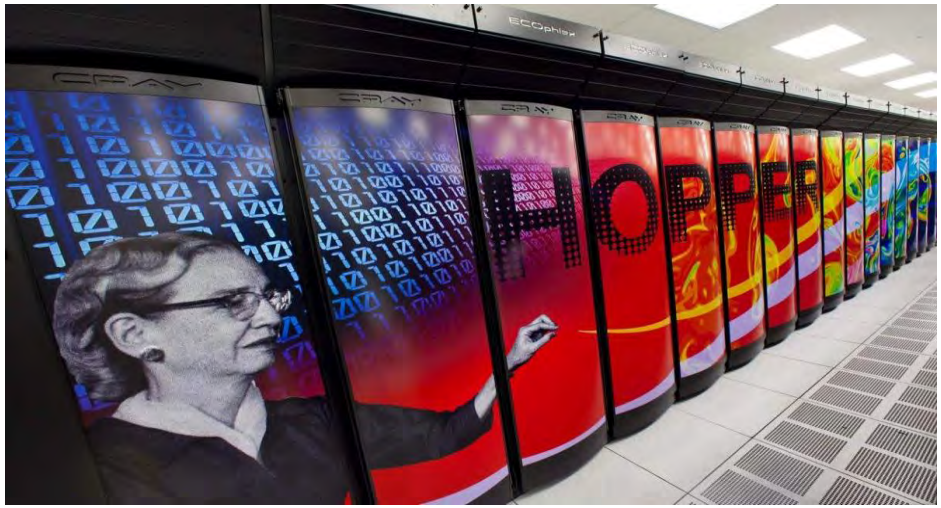
U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC-6 Project Successfully Concluded

- **NERSC-6 (Hopper) Project Closeout Report finalized in August 2011.**
- **Project was very successful:**
  - Exceeded SOW performance goal of 70 – 100 TFlop/s SSP vs. Actual 143.79 TFlop/s SSP
  - Under the budget
  - 7 months ahead of schedule

Here she is!

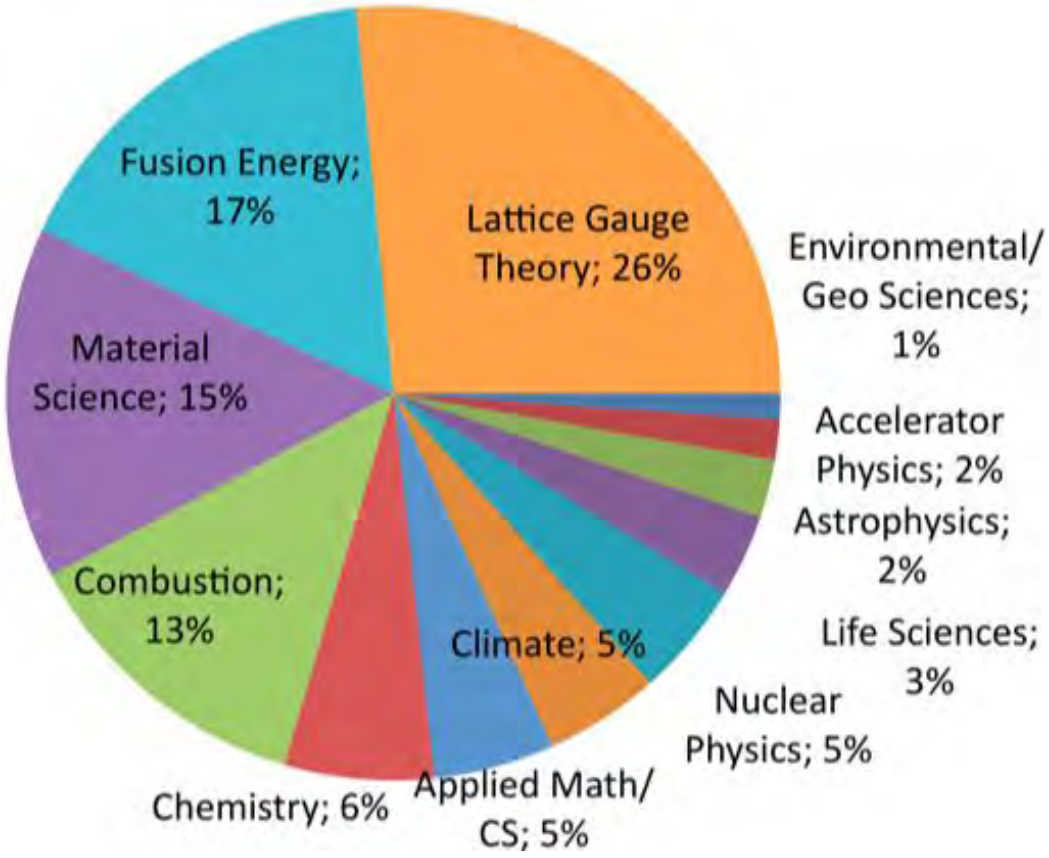
- **5 months of Early User Period for testing Hopper (shared with Cray engineers)**
- **Hopper went into production and started charging on May 1, 2011**



Hopper Early User Hours

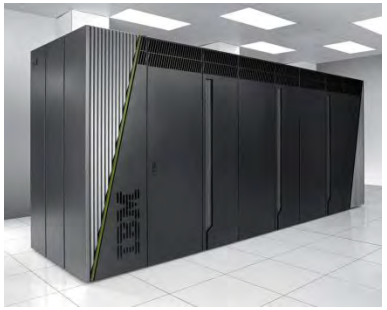
- ~320 million early hours delivered to science offices
- ~280 projects have used time
- ~1,000 users have accessed the system
- Consistently 300-400 unique users logged into system at any time
- Top Offices: BES (33%)–NP (20)-FES (17)-HEP (16)-BER (9)-ASCR(5)
- Top Users: Chen (BES 40M), Toussaint (HEP 40M), Savage (NP 31M), Ching (BES 24M), Pindzola (FES 19M), Chang (FES 19M)

Breakdown of Early User Hours by Science Area
Nov 2010 – May 1st 2011



Leadership Computing Facilities Progress

- **ALCF**
  - On site Operational Assessment: August 25-25, 2011
- **OLCF**
  - Revised Current Plan of Record
    - Upgrading Jaguar rather than acquiring new machine
      - Phase 1: Upgrade processors (AMD Interlagos) and interconnect (Gemini) in all 200 cabinets; Add Nvidia Fermi+ accelerator chips to 10 cabinets
      - Phase 2: Depending on budget, add Nvidia Kepler accelerator chips to 72-200 cabinets
  - Mini Lehman Review: August 16, 2011 recommended
    - Approval of project baseline
    - Finalizing contract



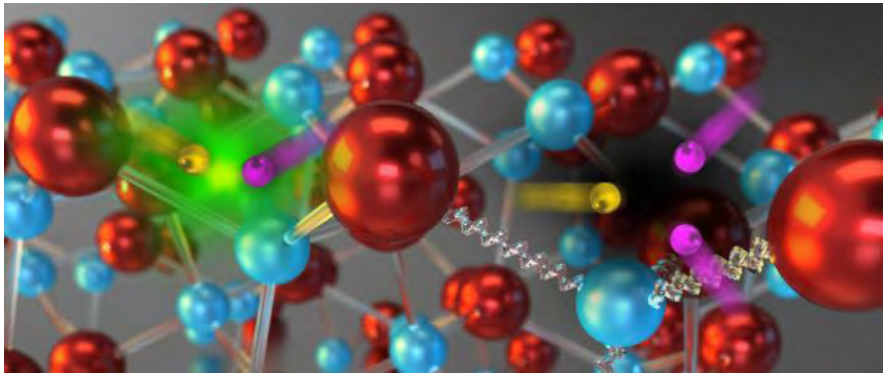
INCITE in Review – Highlights scientific accomplishments at ALCF and OLCF
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/INCITE_IR.pdf

Energy Sciences Net

NERSC Users Making Breakthrough on More Efficient LED Lighting (BES)

- **LEDs are up to 3x more energy efficient and last 10x longer than fluorescent lights but**
  - *"LED droop" makes them unusable for lighting rooms, since efficiency drops when current is scaled.*
- ***Science discovery: Root of the problem is Indirect Auger recombination combined with carrier scattering***
- **Implication: allowing university and industry researchers to work on solutions.**

1.3 M hours w/ up to 9,412 cores on Franklin, Carver, and Hopper. NERSC NISE award.

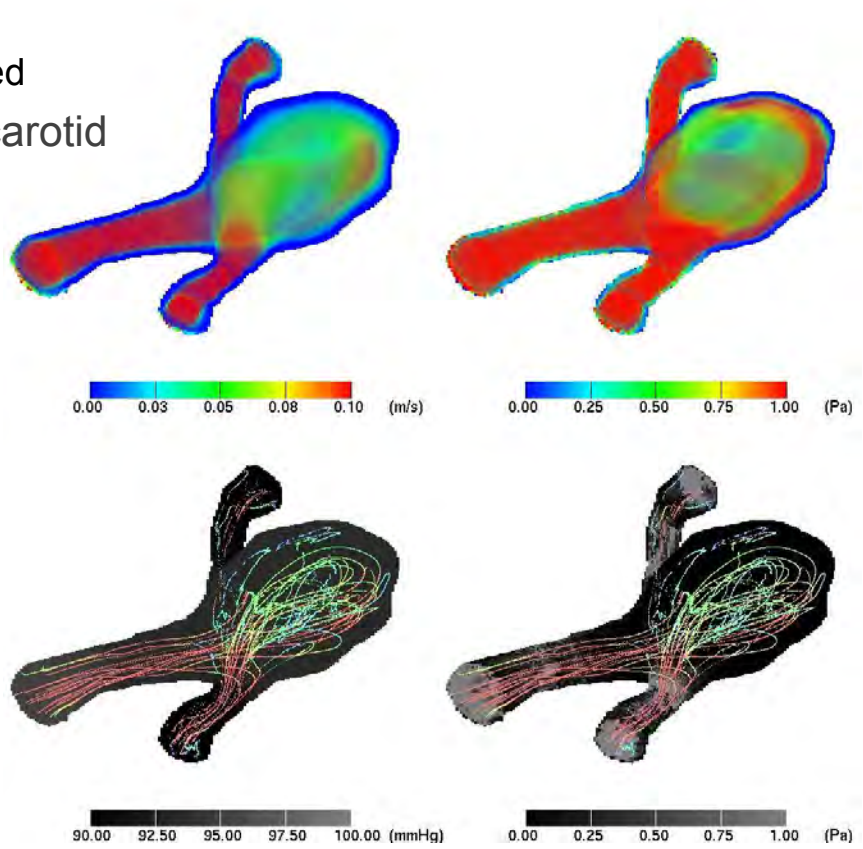


E. Kioupakis, C. Van de Walle (UC Santa Barbara)

Schematic of an LED crystal. At left, an electron and electron hole recombine and release light. In Auger recombination (right) the electron and hole combine with a third carrier, releasing no photon. The energy loss is also assisted by indirect processes, vibrations in the crystal lattice shown as squiggles.

Whole-Brain Blood Flow Simulations

- **INCITE, PI Peter Coveney (University College London)**
  - HemeLB: Sparse-geometry, optimized Lattice Boltzmann code
    - Standalone mode or dynamically steered
  - Studied three patient-specific internal carotid artery aneurysms
    - Starts with input of angiography data
      - Standalone mode on Intrepid



IMPACT

- Improve diagnosis and treatment of aneurysms
  - Dynamically steered

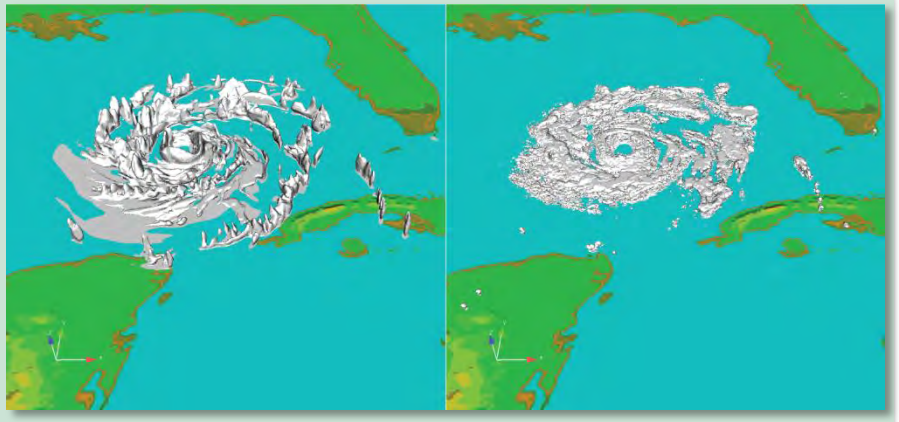
ALCF Contribution

Intrepid allows flow calculation at speeds fast enough to be clinically useful

Supercomputers and Airplanes Help Model Hurricane Structure and Intensity

Scientists predict disaster with models, high-performance computing, and perfect storms

- A research team led by Jon Reisner of LANL is employing Jaguar to use data from lightning detectors and even wind instruments mounted on planes flown into the eye of a hurricane to improve atmospheric models.
- These simulations may lead to more accurate prediction of hurricane intensities and better preparation of the public for these inevitable disasters.
- Reisner's team is using an atmospheric science model developed at LANL called HIGRAD to simulate and track individual liquid or solid particles on a nanometer scale.
- In total, HIGRAD used approximately 118,000 Jaguar processors during three separate simulations.
- Beyond refining the models, researchers discovered that traditional models are plagued with improper expression of cloud boundaries.



Two Hurricane Rita simulations use different numerical methods. The Reisner group's HIGRAD code can simulate both liquid and solid elements in either a Lagrangian framework (right panel) using a particle incell approach or the more typical Eulerian cloud modeling approach (left panel). Differences between the two approaches are the result of numerical errors produced by the Eulerian cloud model due to its inability to accurately resolve the movement of sharp cloud boundaries such as those occurring near the hurricane eye wall. Image courtesy of Jon Reisner, Los Alamos National Laboratory

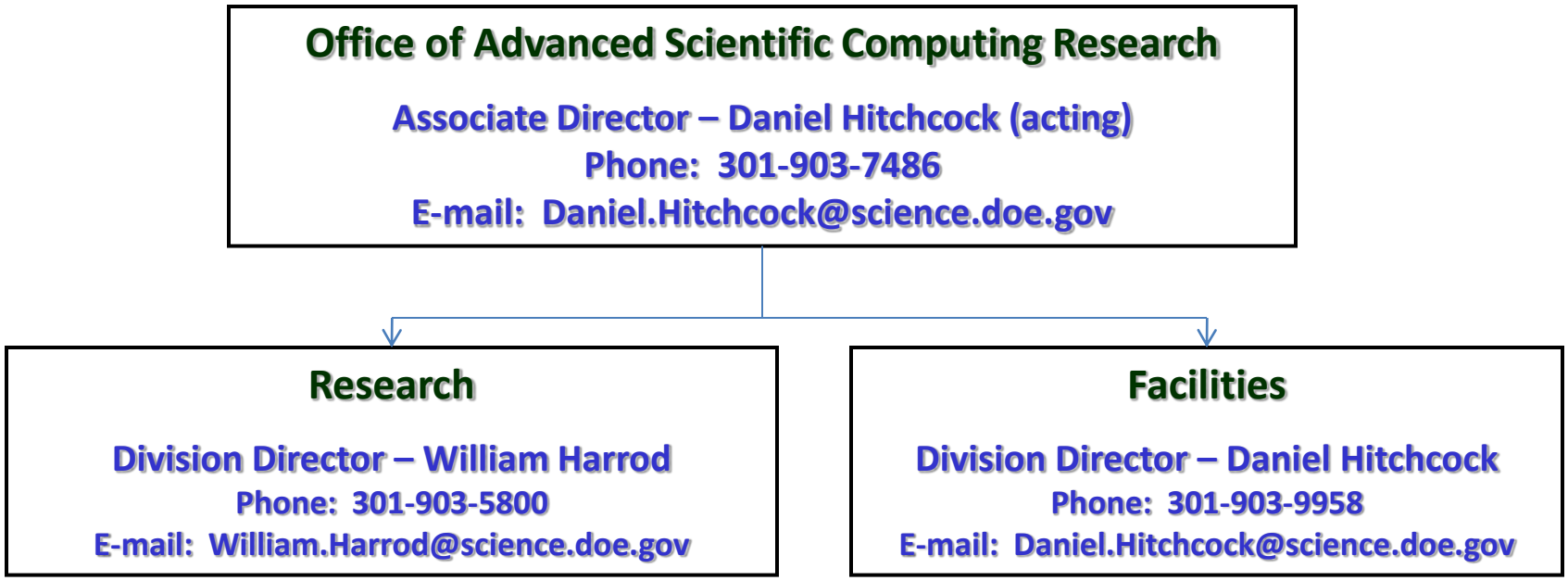
"Long term what we want to do is use the lightning data, like we used the radar data, to help understand how much energy is being released in a hurricane at a given time. And that hopefully will lead to much better predictions of intensification," – PI Jon Reisner

New ASCR Staff

Computer Scientist – Lenore M. Mullin

Lenore has a BS in Mathematics from SUNY New Paltz, and an MS in Solids State Physics and Materials Science as well as a PhD in Computer Science from Syracuse University. She received a NYS Science and Technology seed grant for her dissertation research entitled A Mathematics of Arrays. She spent 3 years at NSF as a Program Officer in CISE CCF Algorithmic Foundations: Numeric and Symbolic Computing. Before coming to NSF she developed courses and curriculum at the undergraduate and graduate level in High Performance Scientific Computing as a tenured professor in the Computer Science Department at the University at Albany, SUNY. Prior to that she was at the University of Missouri-Rolla where she was awarded the NSF Presidential Faculty Fellowship entitled Intermediate Languages for Enhanced Parallel Performance. Prior to her academic career she was a Research Technical Staff member in the APL Design Group at IBM TJ Watson Research Center working with Ken Iverson. She has numerous published articles and a patent with IBM on indexing patterned sparse arrays for microprocessor data caches. She has also received research funding from NSERC and NSF throughout her career.

ASCR at a Glance



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/