U.S. DEPARTMENT OF ENERGY | Office of Science

DOE/SC ASCR and Exascale

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Senior Advisor

Advanced Scientific Computing Research

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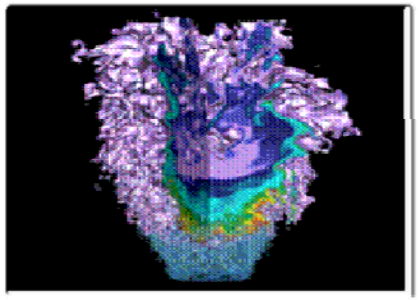
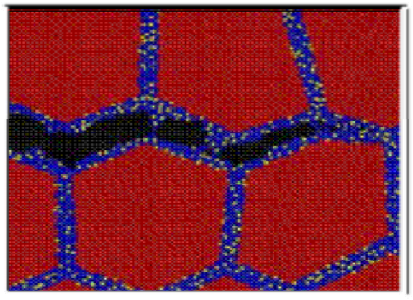
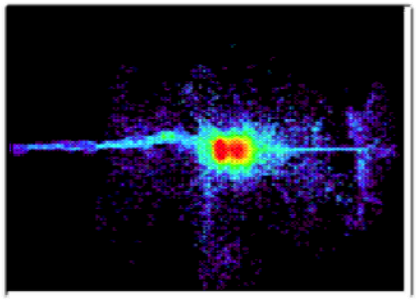
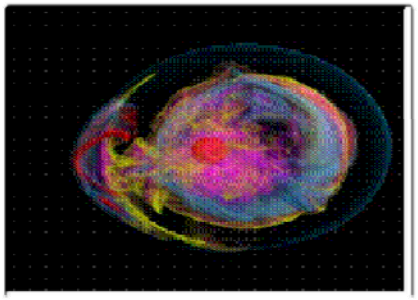
Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

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:

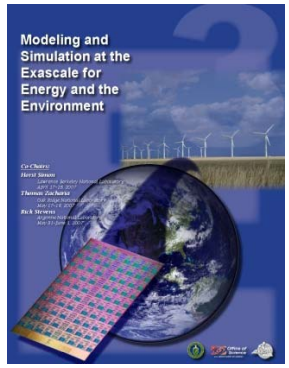
- Research in uncertainty quantification for drawing predictive results from simulation
- Co-design centers to deliver next generation scientific applications by coupling application development with formulation of computer hardware architectures and system software.
- Investments in U.S. industry to 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.

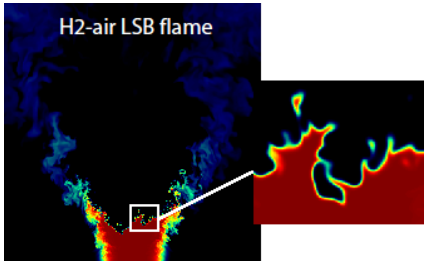





Why Exascale -- Exascale Applications and Technology

http://www.science.doe.gov/ascr/WorkshopsConferences/GrandChallenges.html

- **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

"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. Failure to initiate an exascale program could lead to a loss of U. S. competitiveness in several critical technologies."

Trivelpiece Panel Report, January, 2010

ASCR Advisory SubCommittee Exascale Report

http://www.science.doe.gov/ascr/ASCAC/Reports/Exascale-Subcommittee-Report.pdf

- **Charge**
  - Assess the opportunities and challenges of exascale computing for the advancement of science, technology, and Office of Science missions
  - Identify strategies that ASCR can use to address the challenges and deliver on such opportunities
- **Findings**
  - The mission and science opportunities in going to exascale are compelling
  - Making he transition to exascale poses numerous unavoidable scientific, algorithmic, mathematical, software, and technological challenges
  - The benefits of going to exascale far outweigh the costs
  - The exascale initiative as described in workshop reports and expert testimony portends an integrated approach to the path forward
- **Recommendation**
  - DOE should proceed expeditiously with an exascale initiative so that it continues to lead in using extreme scale computing to meet important national needs.

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. *ASCAC subcommittee report*

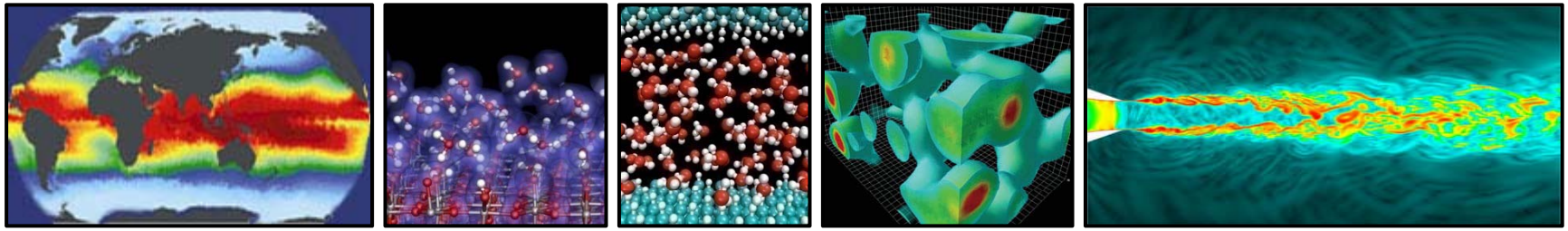
Investments for Exascale Computing
Opportunities to Accelerate the Frontiers of Science through HPC

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:

- Leverage new chip technologies from the private sector to bring exascale capabilities within reach in terms of cost, feasibility, and energy utilization by the end of the decade;
- Support research efforts in applied mathematics and computer science to develop libraries, tools, and software for these new technologies;
- Create close partnerships with computational and computer scientists, applied mathematicians, and vendors to develop exascale platforms and codes cooperatively.

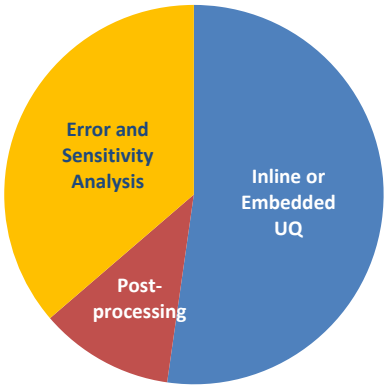


DOE/ASCR Progress toward Exascale

- **FY2010 Proposals processed in Exascale related topic areas:**
  - **Applied Math:** Uncertainty Quantification
  - **Computer Science:**
    - Advanced Architectures
    - X-Stack
    - Scientific Data Management and Analysis
- **FY 2010 Proposals still under review**
  - **Computational Partnerships:** Co-Design (21 Proposals requesting ~ $160M/year)
- **Exascale Coordination meetings with other Federal Departments and Agencies**
- **Formalizing Partnership with National Nuclear Security Administration (NNSA) within DOE through Memorandum of Understanding**

ASCR's Exascale Portfolio

Uncertainty Quantification

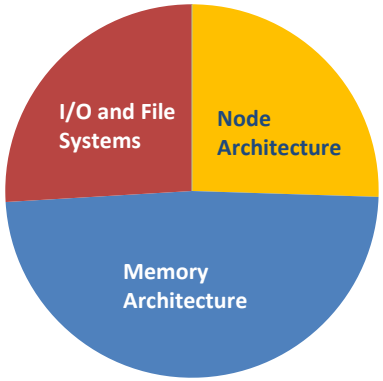


90 proposals received requesting ~$45M/year

6 funded at $3M/yr

60% Laboratory
40% University

Advanced Architectures

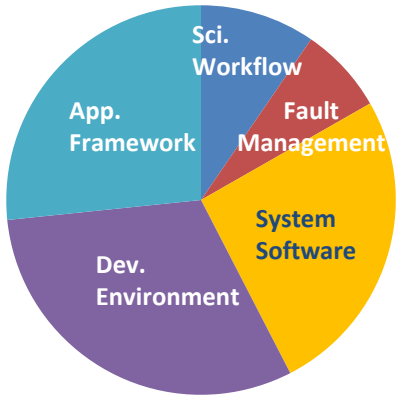


28 proposals received requesting ~$28M/year

6 funded at $5M/year

60% Laboratory
40% University and Industry

X-Stack

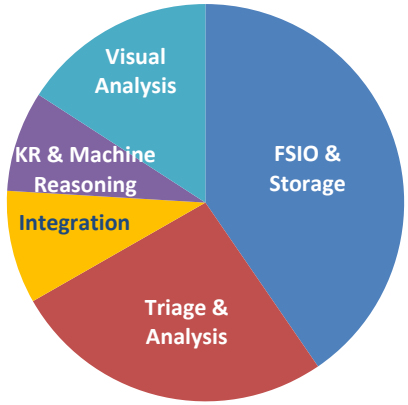


55 proposals received requesting ~$40M/year

11 funded at $5M/year

50% Laboratory
50% University and Industry

Scientific Data Management & Analysis



37 proposals received requesting ~$2M/year

11 funded at $5M/year

60 % Laboratory
40% University and Industry

ASCR Exascale Research Kick-off Meeting

- **PI meeting for**
  - Advanced Architecture, X-Stack, Scientific Data Management and Analysis at Extreme Scales awardees
  - Co-Design planning grant recipients
- **Expected Outcomes:**
  - Awareness **within** each solicitation communities and ASCR what members are doing and areas where they can leverage and supplement their work
  - Awareness **across** solicitation communities of what is going on and where each project fits in relation to the broad spectrum
  - Identification of gaps in ASCR exascale research potfolio
  - Lay groundwork for collaboration/cooperation with NNSA Exascale Roadmapping activities

The Exascale PI meeting
Facilitated & Choreographed

- Monday afternoon: ASCR presentations
- Tuesday – Wednesday morning: 3 poster sessions
  - each project representative made a 5-minute intro to the poster prior to poster session; project teams were to use poster sessions for networking
- Wednesday Afternoon: working groups to identify crosscutting topics + outbrief
  - Each attendee was assigned to one of 8 Working Groups;
  - Each WG was moderated by an NNSA facilitator and had a student scribe to take notes; two ASCR PIs served as reporters and presented working group outbrief
- Wednesday dinner: ASCR & NNSA program offices identify five main topics
- Thursday: further discussions of crosscutting topics + outbrief
  - Morning: definition & interrelations (in same working group)
  - Afternoon: issues (in self-identified working groups)
- Friday: gap analysis
  - Each attendee was assigned to a different WG
- In addition, there were homework assignments
  - Exascale Research Coverage Assessment
  - Dance cards
- Results are being tabulated

Five Crossing cutting topics identified from working groups:

- Programming Models
- Resilience and Fault Tolerance
- Data Management & I/O Architecture
- Memory / Data Movement and Energy Efficiency
- Application Architecture

Homework Assignments

Forms Filled in as participants visited posters

Exascale Research Coverage Assessment Name: _____

Issues	Importance (Hi/Med/Lo)	Coverage in ASCR FOAs (Yes / No)	Coverage in ASCR Exascale Projects (Adequate/Inadequate)	Coverage by Other Agencies' Projects (Agency & Project Title)
Hardware Architecture and I/O				
Fault detection and resilience				
File systems and I/O				
Memory systems				
Power management				
Simulators				
Synchronization				
Testbeds				
Other:				

Used to Identify Priorities and Gaps

Dance Cards

Used to Foster Collaborations

ASCR Project / Lead PI	Poster Session	Priority (Hi/Med/Lo)	Likely Nature of Collaboration and Timeframe
Advanced Architectures and Critical Technologies for Exascale Computing			
Blackcomb (Vetter)	2 Tues pm		
CODES (Ross)	3 Wed am		
CoDEx (Shalf)	1 Tues am		
DMD (Rodrigues)	3 Wed am		
NoLoSS (Ross)	2 Tues pm		
Thrifty (Torrellas)	1 Tues am		

POCs

ASCR CS Program Managers: Lucy Nowell, Sonia Sachs

Meeting material at
http://exascaleresearch.labworks.org/ascr2011

ASCR at a Glance

Relevant Websites

ASCR: science.doe.gov/ascr/

ASCR Workshops and Conferences:
science.doe.gov/ascr/WorkshopsConferences/WorkshopsConferences.html

SciDAC: www.scidac.gov

INCITE: www.science.doe.gov/ascr/incite/

Exascale Software: www.exascale.org

DOE Grants and Contracts info: science.doe.gov/grants/