U.S. DEPARTMENT OF ENERGY | Office of Science

# View from Germantown

August 14, 2012

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

# *Context Within DOE and SC*


## ASCR Contributes to DOE's Goal to

Maintain a vibrant U.S. effort in science and engineering as a cornerstone of our economic prosperity with clear leadership in strategic areas.

- Lead Computational Sciences and High-Performance Computing
  - **Targeted Outcome:**
    - Continue to develop and deploy high –performance computing hardware and software systems through exascale platforms.

# *Advanced Scientific Computing Research*

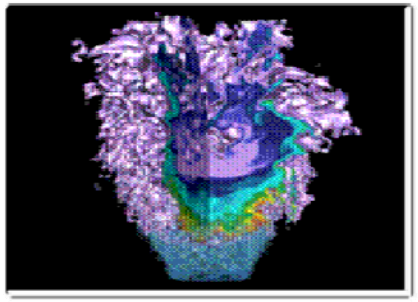
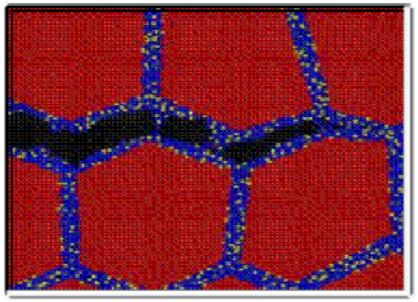
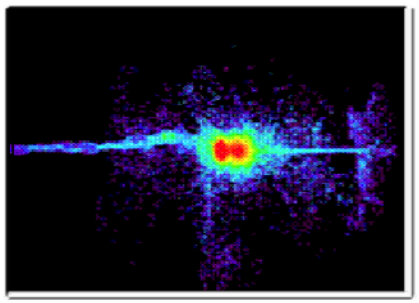
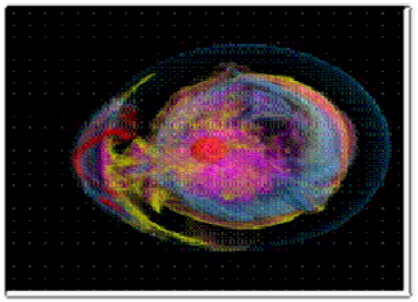
Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

## 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.

# The Growing Importance of Data

- President Obama announces Big Data Initiative on March 29, 2012
- All of the exascale hardware trends impac data-intensive science (in many cases more than compute-intensive applications Square Kilometer Array in Australia needs 100 MW for compute infrastructure;
- 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;

Office of Science and Technology Policy
Executive Office of the President
New Executive Office Building
Washington, DC 20502

FOR IMMEDIATE RELEASE
March 29, 2012

Contact: Rick Weiss 202 456-6037 rweiss@ostp.eop.gov
Lisa-Joy Zgorski 703 292-8311 lisajoy@nsf.gov

**OBAMA ADMINISTRATION UNVEILS "BIG DATA" INITIATIVE: ANNOUNCES $200 MILLION IN NEW R&D INVESTMENTS**

Aiming to make the most of the fast-growing volume of digital data, the Obama Administration today announced a "Big Data Research and Development Initiative." By improving our ability to extract knowledge and insights from large and complex collections of digital data, the initiative promises to help solve some the Nation's most pressing challenges.

To launch the initiative, six Federal departments and agencies today announced more than $200 million in new commitments that, together, promise to greatly improve the tools and techniques needed to access, organize, and glean discoveries from huge volumes of digital data.

"In the same way that past Federal investments in information-technology R&D led to dramatic advances in supercomputing and the creation of the Internet, the initiative we are launching today promises to transform our ability to use Big Data for scientific discovery, environmental and biomedical research, education, and national security," said Dr. John P. Holdren, Assistant to the President and Director of the White House Office of Science and Technology Policy.

To make the most of this opportunity, the White House Office of Science and Technology Policy (OSTP)—in concert with several Federal departments and agencies—created the Big Data Research and Development Initiative to:

- Advance state-of-the-art core technologies needed to collect, store, preserve, manage, analyze, and share huge quantities of data.
- Harness these technologies to accelerate the pace of discovery in science and engineering, strengthen our national security, and transform teaching and learning; and
- Expand the workforce needed to develop and use Big Data technologies.

- 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).

# 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 |
| Exascale / Big Data — Computer Science | 47,301 | 47,400 | 54,580 | + 7,180 |
| Exascale / Big Data — Computational Partnerships (includes SciDAC) | 52,813 | 44,250 | 56,776 | + 12,526 |
| Big Data — Next Generation Networking for Science | 12,313 | 12,751 | 16,194 | + 3,443 |
| 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 |
| Leadership Computing Facilities | 158,020 | 156,000 | 145,000 | -11,000 |
| Exascale — Research and Evaluation Prototypes | 4,301 | 30,000 | 22,500 | - 7,500 |
| High Performance Network Facilities and Testbeds (ESnet) | 30,451 | 34,500 | 32,000 | - 2,500 |
| 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**[a/] | **440,868** | **455,593** | **+14,725** |

- Math for data-intensive science
- Computer Science challenge of big data
- Co-design center and partnerships for data-intensive science
- Networking challenges of data-intensive science
- Supports site prep. for new NERSC bld.
- Reduce infrastructure investments
- Focus vendor partnerships and critical technologies
- Supports staged production deployment of 100Gbps optical ring

[a/] Total is reduced by $11,680,000 $10,428,000 of which was transferred to the Small Business Innovation Research (SBIR) program, and $1,252,000 of which was transferred to the Small Business Technology Transfer (STTR) program.

# FY13 ASCR HEWD Mark

**The Advanced Scientific Computing Research (ASCR) program develops and hosts some of the world's fastest computing and network capabilities to enable science and energy modeling, simulation, and research. The Committee recommends $442,000,000 for Advanced Scientific Computing Research, the same as fiscal year 2012 and $13,593,000 below the request.**

***Exascale Computing.*—The Committee continues to support the exascale initiative, which seeks to develop the next generation of computing systems three orders of magnitude faster than today's fastest systems. This decade-long effort is critical to enabling basic and energy-focused science research not previously possible and to maintaining the nation's global leadership in computing technologies.**

**In the fiscal year 2012 conference report, the Department was directed to submit a detailed joint Science-NNSA exascale plan by February 10, 2012. This report, which would provide context for long-term resource planning and prioritization, still has not been submitted as of early April 2012. The Department was made aware of the reporting requirement after the House and Senate Committees completed consideration in June and September of 2011, respectively, and there has been ample time for preparation since. While the Committee appreciates the efforts within the Office of Science to draft the report, it remains concerned that such an extended approval process is necessary to summarize the programmatic outline of a central feature of the Department's computing programs. The Administration should not further delay the report's formal submittal due to a drawn-out concurrence process.**

**The budget request highlights data-intensive computing as a necessary enabler for exascale systems and calls out work in this area separately from the exascale initiative. The Committee expects that the Department has integrated into the exascale report any plans for work on computing challenges related to data-intensive science.**

***Leadership Computing.*—In addition to the long-term exascale initiative, the Committee supports continued upgrade and operation of the Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories and of the High Performance Production Computing capabilities at Lawrence Berkeley National Laboratory. These systems' capabilities are a critical component of science and industrial research and development across the nation, and they should be maintained as world-leading facilities.**

# FY13 ASCR SEWD Mark

**The Committee recommends $455,593,000 as requested for Advanced Scientific Computing Research. Within these funds, the Committee recommends $68,500,000 as requested for the exascale initiative to spur U.S. innovation and increase the country's ability to address critical national challenges.**

**The Committee also recommends $94,000,000 for the Oak Ridge Leadership Computing Facility to move forward with upgrades to its Cray XT5 with a peak capability of more than 20 petaflops, $67,000,000 for the Argonne Leadership Computing Facility to move forward with upgrades to its IBM Blue Gene/P systems with a peak capability of 10 petaflops, $68,105,000 for the National Energy Research Scientific Computing Center facility at Lawrence Berkeley National Laboratory to support operations and infrastructure expenses for the new Computational Research and Theory Building, and $35,000,000 to help support extended deployment of a 100 gigabit-per-second network to the national laboratories. Having high end open science computing will not only help the United States maintain leadership in computing and develop breakthroughs that will improve the everyday lives of our citizens through new technologies available to them, but will also support breakthroughs in the other research areas in the Office of Science. Research programs such as fusion energy science, biofuels, and materials by design all stand to benefit from investments in open science computer modeling and simulation.**

**The Committee recommends that up to $8,000,000 shall be available to pursue data-intensive science, but the Committee directs the Office of Science to develop a plan that explains the extent of the problem, how research efforts will address data analysis problems, and the funding needed to overcome these data challenges.**

**The Committee encourages the Office of Science to continue working with small- and medium-sized manufacturers and businesses to educate them about the benefits of using high performance computing for modeling and simulations to solve tough manufacturing and engineering challenges and reduce development costs. The Committee also encourages the Office of Science to simplify software and codes so a broader set of businesses can take advantage of these powerful tools.**

# FY13 ASCR Appropriations: HEWD vs. SEWD

## HEWD Mark (in thousands)

| | FY 12 Enacted | FY 13 Request | FY 13 House | FY 13 House vs. FY 12 Approp. | | FY 13 House vs. FY 13 Request | |
|---|---|---|---|---|---|---|---|
| ASCR Total | 440,868 | 455,593 | 442,000 | 1,132 | 0.26% | -13,593 | -2.98% |
| Research | 154,565 | 182,620 | 164,161 | 9,596 | 6.21% | -18,459 | -10.11% |
| Facilities | 286,303 | 272,973 | 277,839 | -8,464 | -2.96% | 4,866 | 1.78% |

- The House language indicated support for Exascale and ASCR Facilities
- It assumes that the plans for data intensive science research have been included in the Exascale plan.

## SEWD Mark (in thousands)

| | FY 12 Enacted | FY 13 Request | FY 13 Senate | FY 13 Senate vs. FY 12 Approp. | | FY 13 Senate vs. FY 13 Request | |
|---|---|---|---|---|---|---|---|
| ASCR Total | 440,868 | 455,593 | 455,593 | 14,725 | 3.34% | --- | ---- |
| Research | 154,565 | 182,620 | 160,443 | 5,878 | 3.80% | -22,177 | -12.14% |
| Facilities | 286,303 | 272,973 | 295,150 | 8,847 | 3.09% | 22,177 | 8.12% |

- The Senate mark identified specific levels of support for Exascale and ASCR Facilities
  - Exascale -- $68.5M
  - NERSC -- $68.1M
  - ALCF -- $67M
  - OLCF -- $94M
- Up to $8M is shall be available for data intensive science but DOE must develop a plan that explains the extent of the problem, how research efforts will address data analysis problems, and the funding needed to overcome these data challenges

# *Proposed DOE High End Revitalization Act of 2012*

- Amends DOE High End Revitalization Act of 2004
  - Includes all of DOE, not just Office of Science
  - Continues support of leadership computing
  - Defines Exascale computing – computing through the use of a computing machine that performs near or above 10 to the 18th power floating point operations
  - Replaces section on Software Institute with section on Exascale computing… The Secretary shall
    - **Conduct a research program** to develop 1 or more exascale computing machines to promote the missions of the Department
    - **Coordinate the development of 1 or more exascale** computing machines across all applicable agencies of the Department
    - Carry out the **program through an integration of application, computer science and computer hardware architecture using public-private partnerships** to ensure that 1 or more exascale computing machines are capable of solving Department target applications and Science applications **(Co-Design)**
    - Development of exascale machines conducted through **merit review**
    - **Submit a report annually** describes funding for exascale computing by functional element of the department

# *ASCR Personnel News*

- Facilities
  - Division Director selection in progress
  - Yukiko Sekine, NERSC Program Director since 2006 is retiring. Served several roles in ASCR including Program Manager for Scientific Visualization and Data Management from 2004-2006
  - Dave Goodwin will be acting NERSC Program Manager

# *Upcoming ASCR Research Job Announcements*

## DOE Applied Mathematics Program Manager

The Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR), is seeking a motivated and highly qualified individual to serve as a Program Manager for Applied Mathematics in its Computational Science Research & Partnerships (SciDAC) Division.

Applicants should have a strong background in applied mathematics and high-performance computing with an understanding of the computational modeling, simulation and analysis issues related to high-performance scientific computing given that numerous significant modifications to today's tools and techniques will be required to deliver on the promise of exascale computing for science.

At this time, this position has not been officially posted. However, interested candidates should monitor the DOE Office of Science jobs site (http://science.energy.gov/about/jobs#program/) and begin gathering the required materials. After the position has been posted, applicants will have to complete information on qualifications and other details. Applicants will need an account on the USAJOBS site (http://www.usajobs.gov/) and it is essential that they are prepared to provide transcripts for graduate and undergraduate education when submitting their application.

•

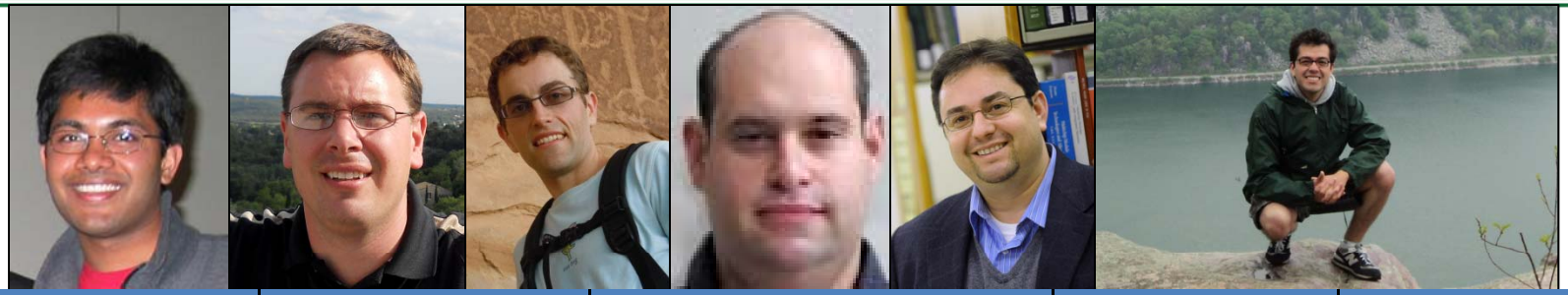
# *Upcoming ASCR Research Job Announcements (cont)*

## DOE Computer Science Program Manager

The Department of Energy, Office of Science, Office of Advanced Scientific Computing Research (ASCR), is seeking a motivated and highly qualified individual to serve as a Program Manager for Computer Science in its Computational Science Research & Partnerships (SciDAC) Division.

The Computer Scientist in this position will help to reinvent the field of Computer Science with respect to operating and runtime systems for extreme scale supercomputing. At this time, this position has not been officially posted. However, interested candidates should monitor the DOE Office of Science jobs site (http://science.energy.gov/about/jobs#program/) and begin gathering the required materials. After the position has been posted, applicants will have to complete information on qualifications and other details. Applicants will need an account on the USAJOBS site (http://www.usajobs.gov/) and it is essential that they are prepared to provide transcripts for graduate and undergraduate education when submitting their application.

# Awards - FY12 ASCR Early Career Research Program



| Name | Institution | Title | Program | Topic Area |
|---|---|---|---|---|
| **Pavan Balaji**<br>**PhD in 2006** | Argonne National Lab | **Exploring Efficient Data Movement Strategies for Exascale Systems with Deep Memory Hierarchies** | Computer Science | Foundations for Exascale Computing |
| **Hank Childs**<br>**PhD in 2006** | Lawrence Berkeley National Lab | **Data Exploration at the Exascale** | Computer Science | Data & Visualization |
| **Aleksandar Donev**<br>**PhD in 2006** | New York University | **Stochastic Simulation of Complex Fluid Flows** | Applied Math | Multiscale Complex Systems |
| **Mattan Erez**<br>**PhD in 2007** | University of Texas at Austin | **Containment Domains: Programming and Execution Model Support for Resiliency** | Computer Science | Runtime Systems and OS |
| **Haim Waisman**<br>**PhD in 2005** | Columbia University | **Regularized Finite Element Formulations for Shear Band Instabilities in Metals** | Applied Math | Multiscale Complex Systems |
| **Victor Zavala**<br>**PhD in 2008** | Argonne National Lab | **Next-Generation Optimization Under Uncertainty: Structure-Oriented Algorithms** | Applied Math | Optimization under Uncertainty |

# *DOE Office of Science*
# *Early Career Research Program*

**FY13 is 4th year of this University & DOE Laboratory funding opportunity:**

- Posted on July 20, 2012
- Pre-applications due Sept 6
- Encourage applications by Oct 4
- Full applications due Nov 26

**The Early Career program supports:**

- Development of individual research programs of outstanding scientists early in their careers
- Stimulates research careers in the disciplines supported by the DOE

http://science.energy.gov/early-career

## ASCR proposals are focused on basic research programs:

- **Applied Math – 3 topic areas**
  - To develop mathematical descriptions, models, methods and algorithms to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales.

  To develop the underlying understanding and software to make effective use of computers at extreme scales
  - To transform extreme scale data from experiments and simulations into scientific insight.

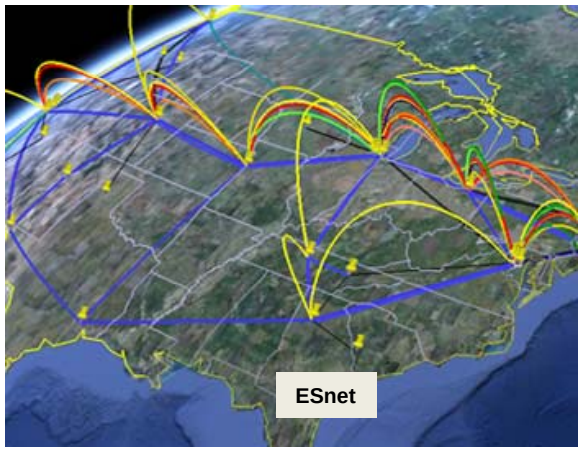
- **Computer Science – 3 topic areas focused on Challenges of Exascale**
  - Programming models, language constructs, compilers and runtime systems that address the challenges of programming applications which are characterized by computations on irregular data structures and with unstructured and dynamic communication patterns;
  - Software solutions that dynamically capture data movement patterns in applications and enable the adaptive selection of optimal data movement strategies, leveraging heterogeneous processors and novel hardware architectures;
  - Scientific data management, including data provenance representation and capture; data integration/fusion; data interoperability; and scientific workflow systems that support data analysis and visualization for petabyte to exabyte data sets.

# *World Class Facilities*

- **NERSC: Hopper, NERSC-7, CRT Building, NRP Power upgrade**
- **ALCF: Mira, Power upgrade**
- **OLCF: Titan, Power upgrade**
- **Energy Sciences Network (ESnet): 100 GigaBits/Sec**

Oak Ridge Leadership Computing Facility

National Energy Research Scientific Computing Center


ESnet

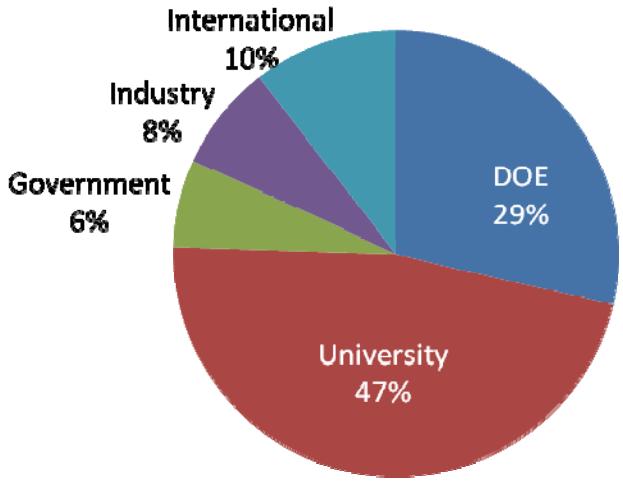
Argonne Leadership Computing Facility

# *Innovative and Novel Computational Impact on Theory and Experiment*

INCITE awards time on the Argonne and Oak Ridge Leadership Computing Facility (ALCF and OLCF) systems for researchers to pursue transformational advances in science and technology.

## 2013 Call for Proposals

- Request for Information helped attract new projects
- Call closed June 27th, 2012
- Total requests ~14 billion core-hours, nearly 3x more than the 5 billion core-hours requested last year
- 143 proposals submitted, an increase of nearly 20% over the 119 proposals submitted last year.
- Awards of ~5 billion core-hours to be announced in November for CY 2013




**Number of 2013 INCITE Submittals by PI Affiliation**

## Reaching out to Researchers

*Nearly 50% of the non-renewal proposals are by new PIs.*

**Contact information**
Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org

# *Argonne Leadership Computing Facility*

- **ALCF-2**
  - Completed
    - 2 racks of BG/Q (01/04/12)
    - 48 racks of BG/Q (04/23/12 – 06/08/12)
    - 48 rack HPL (07/14/12)
  - Next steps
    - Preparation for acceptance
    - 2 weeks early science testing before acceptance
    - 1 month of acceptance testing
    - Early science program

- **ALCF-3 Power and Cooling Upgrade**
  - Support upgrade planned for FY16/17
  - CD-0 signed 07/02/12
  - Scope
    - High voltage electrical supply and supporting infrastructure equipment (e.g. transformers, feeders, duct bank, switchgear, etc.)
    - Medium voltage electrical distribution and supporting infrastructure equipment (e.g. transformers, switchgear, panel boards, etc.).
    - Air and water cooling systems.
    - Argonne's central campus cooling water systems.

See Early Science Presentation by Paul Messina's

# *Oak Ridge Leadership Computing Facility*

- **OLCF-3 "Titan" Project Status**
  - Completed phase 1 upgrade of Jaguar to 16-core processors, doubled system memory, and new interconnect, on schedule in February 2012
  - Phase 2: Adding 20 PF of NVIDIA "Kepler" GPUs to system beginning Oct. 2012
  - Aggressive goal is to have upgraded system available to users in Q1 2013

See Early Science presentation by Bronson Messer

- **Facility**
  - Added 3.3 MW transformer for Titan
  - Approved Mission Need Statement (CD-0) on July 30, 2012 for 20 megawatt power and cooling upgrade
  - Alternatives Analysis and Project Baseline in 2013 with Start of Construction in 2014
  - New capability will allow Titan to overlap operation of OLCF-4 system in 2016/2017
  - Exploring "Lake Water" cooling option

| Titan Specs | |
|---|---|
| Compute Nodes | 18,688 |
| Login & I/O Nodes | 512 |
| Memory per node | 32 GB + 6 GB |
| # of Fermi chips (2012) | 960 |
| # of NVIDIA K20 "Kepler" processor (2013) | 14,592 |
| Total System Memory | 688 TB |
| Total System Peak Performance | 20+ Petaflops |

# *NERSC Upgrades*

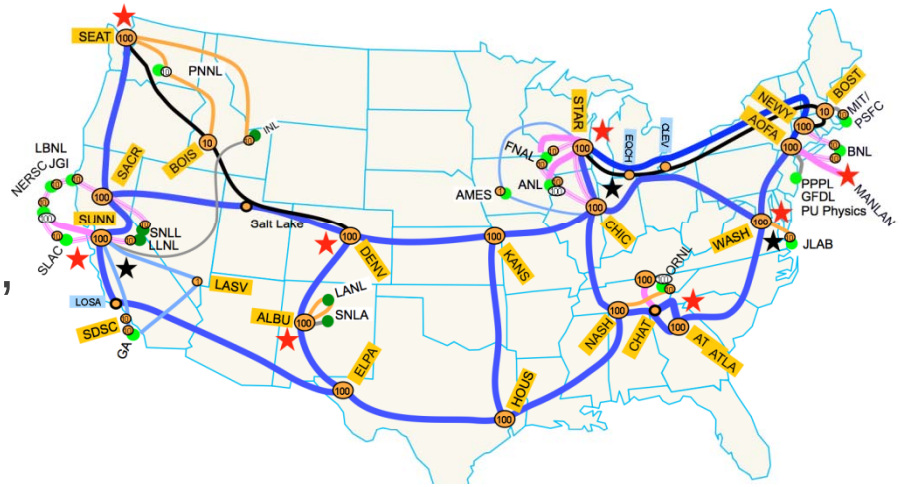
- **The $53 million NERSC-7, a ~2PF Cray Cascade,**
  - CD-3 approved in June, 2012
  - The contract with Cray was signed in June
  - Delivery Expected in 2014


- The $20 million NERSC Relocation Project at the University of California funded Computational Research and Theory Building will provide 12 MW power and cooling for future NERSC computing resources.

- The > 10 PF (peak) **NERSC-8** upgrade advanced conceptual design to be initiated at the beginning of FY13.

# *ESnet5: World's First Continental 100G Network Moves to Full Production Status*

- Two years of planning, design, and development will culminate in deployment of production 100G network to support DOE science missions, November 2012.
- 20-step build process now underway.
  - ✓ deploying optical components, 100G routers, and other infrastructure on a national footprint
- For the latest information about this transition, please visit: https://my.es.net/esnet5/timeline



# *ESnet Key Accomplishments*

## Organizational Progress

- Inaugural meeting of ESnet Policy Board
- Scientific Networking Division created at Berkeley Lab as new home to ESnet
- Greg Bell named Division Director and Head of ESnet

## Network Innovation

- 100G prototype completed connecting DOE supercomputing sites to major int'l exchange points
- 100G testbed goes live, supporting over 20 active research projects, scheduled 24x7
- OSCARS virtual circuit software version 0.6 released

## Scientific Impact

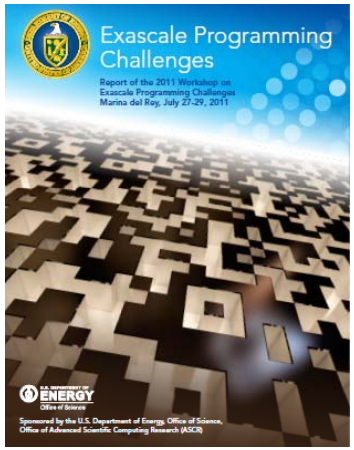
- Network supported major scientific discoveries at LHC, Daya Bay Neutrino Experiment, Palomar Transient Factory

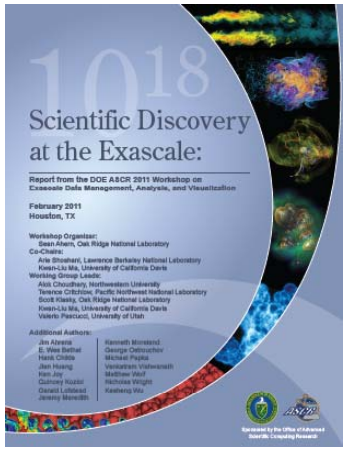
## Community Support

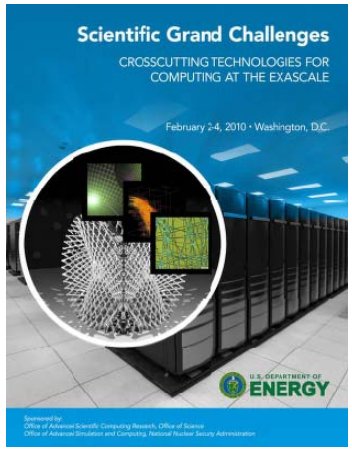
- MyESnet portal launched, provides real-time visualizations of ESnet sites' traffic
- New NSF CI program funds universities to build ESnet-developed Science DMZ model
- Software-Defined Networking focus day organized by ESnet for Summer 2012 Joint Techs
- IPv6 dashboard launched highlighting ESnet connected-sites' v6 deployment status

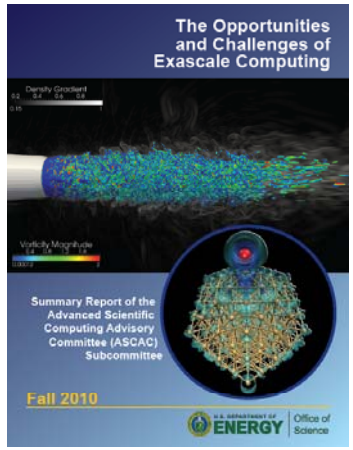
# *Research to Enable the Future*

- Applied Mathematics: Expanding to cover complex systems, uncertainty quantification, large data, exascale algorithms;
- Computer Science: Exascale Computing and Data, Advanced Architectures, Many-core, power aware,…;
- Partnerships: CoDesign to pioneer the future of scientific applications;
- Next Generation Networks for Science: Tools for the future of distributed science



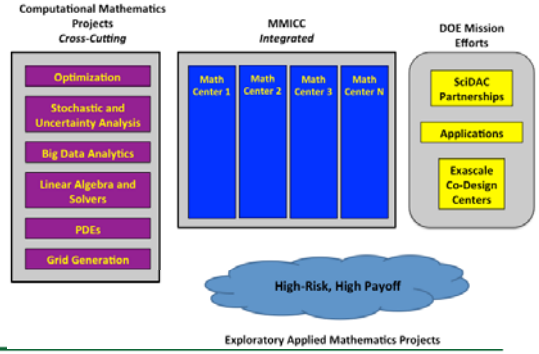



# *Mathematical Multifaceted Integrated Capability Centers (MMICCs) Update*

- Solicitation for "Mathematical Multifaceted Integrated Capability Centers (MMICCs)" released April 4, 2012 - open to DOE National Labs, Universities, and Industry:
  - Address the *long-term mathematical challenges* for one or more DOE grand challenges and that require new integrated, iterative processes across multiple mathematical disciplines.
  - Have *impact* to the DOE mission *in the 5-10+ year timeframe.*
- Distributed to all current DOE Applied Math PIs, NA-Digest, SIAM-SC, SIAM-CSE, and SIAM-OPT list-servers
- Presentation at ASCAC (3/28/2012) and SIAM Committee on Science Policy (4/25/2012)
- Pre-applications were required and due on April 30, 2012
- Full proposals were due June 1, 2012
- In process of negotiating awards



# *Next Generation Networking for Science Scientific Collaboration FOA*

- Program Goal
  - Facilitate complex scientific research team activities through common architectures and protocols, methodologies, workflows, and related technologies
- 70 Proposals Received  (36 unique)
  - 38 from Labs, 32 from Universities
  - 34 unique proposals reviewed in 3 panels
  - 2 proposals declined as out-of-scope
- 10 Proposals Funded
  - 6 Lab lead
  - 4 University lead
  - 8 collaborative teams
  - 2 individual investigator
- Total funding with HEP and FES partners
  - $13.9M ASCR
  - $1.1M HEP and FES

# *Partnerships to Transform the Present*

- SciDAC Institutes: FASTMath, QUEST, SUPER, SDAV
- Strategic ASCR – SC Program Partnerships;
- Computational Science Graduate Fellowship Program: Training the next generation of leaders;
- Workshops to define needs: Joint ASCR – BES workshop on data, Joint ASCR HEP workshop on GEANT4, ASCR ESnet Requirements Workshops, ASCR NERSC Requirements workshops;
- Industrial Outreach through INCITE;
- ASCR SBIR Topic on HPC Software;

See the SciDAC Update presented by Randall Laviolette and Steven Lee

# *Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery Workshop*

**Workshop Goal:** To identify current and anticipated issues in the acquisition, analysis, communication and storage of experimental data in basic energy sciences and to create the foundation for information exchanges and collaborations among ASCR-BES research and facilities communities to address these issues.
**Expected Outcome:** A report that outlines the paths forward to address identified issues based on expected advances in the state of the art in systems, algorithms and processes on the critical path for extracting discoveries from data.

- **Co-sponsored by ASCR and BES**
- **Held:** October 24-25, 2011, Bethesda MD
- **Co-chairs:** Peter Nugent (LBNL), J. Michael Simonson (ORNL)
- **80 Participants from National Laboratories, Universities, NIST, NSF & International**
- **Workshop Website:** https://www.orau.gov/dataworkshop2011/default1.htm

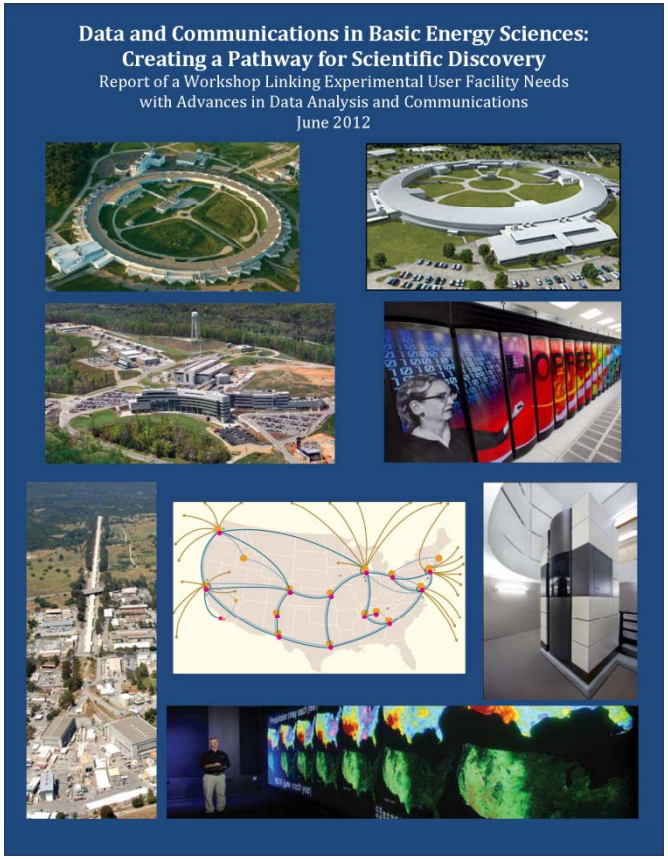
# *Data and Communications in Basic Energy Sciences: Workshop Recommendation Summary*

Focus on high-value-added areas:

- Integrate theory and analysis components seamlessly within experimental workflow.
- Move analysis closer to experiment.
- Match data management access and capabilities with advancements in detectors & sources.

Continue dialog and collaboration between BES and ASCR on areas of interest and benefit

Maximize scientific impact from existing and enhanced user facilities




Workshop report now available at:
http://science.energy.gov/~/media/ascr/pdf/research/scidac/ASCR_BES_Data_Report.pdf

# *Transforming Geant4 for the Future Workshop*

**Background:** Geant4, a software toolkit developed for the simulation of particle-matter interactions, has widespread use in experimental HEP research. Transitioning the code to new computer architectures will increase its performance, allow the incorporation of additional physical models and facilitate handling of the exponentially increasing volume of experimental and simulation data.

**Goal:** To identify applied mathematics and computer science challenges in the effective transformation of Geant4 and to examine opportunities for discovery to meet these challenges.

**Expected Outcome:** A report that outlines a plan forward that will enable Geant4 to thrive in the emerging computing environment.

- **Co-sponsored by ASCR and HEP**
- **Held:** May 8-9, 2012, Rockville MD
- **Co-chairs:** Bob Lucas (USC) and Rob Roser (Fermilab)
- **40 Participants from National Laboratories, Universities & International**
- **Workshop Website:** http://www.orau.gov/transformwkshop2012/

**Consensus:** ASCR and HEP communities must work together to leverage the existing expertise and to initiate new efforts to transform Geant4.

Workshop report will be available soon

# *Investments for Exascale Computing*

## Addressing Critical Challenges to Deliver Predictive Science and Engineering

### Challenges of Exascale

DOE must invest in partnerships and research to address the challenges of emerging hardware to maintain our world-leading position.

- Reduce power requirements by a factor of 10.
- Improve reliability so that hardware operates effectively through component failures.
- Develop tools and techniques to make these advanced systems easier to use.

### Broad Impacts

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.

### The program will:

### Advance all DOE missions

- DOE missions include challenges for which experiments are too risky or expensive to pursue. Exascale capabilities will deliver an new level of precision and predictability to these efforts.

### Drive innovation generally

- Achieving the power efficiency, reliability, and programmability goals essential for exascale will have enormous impact on business information technology, scientific computing, and engineering design at all scales.

### Build on our successes

- DOE is the U.S. leader in delivering extreme scale science and engineering applications on state-of-the-art hardware.

# *ASCR 2012 Exascale Funding*

- Exascale Total is $73.4M in FY12, details:
  - $ 5M in Applied Mathematics for Uncertainty Quantification
  - $20M in Computer Science for Software Environments
    - Including a second round of X-stack projects focused on programming challenges, runtime systems and tools
  - $ 5M in Computational Partnerships for Software Environments
  - $30M in Research and Evaluation Prototypes for Industry Partnerships
    - Includes funding for Fast Forward projects funded through Lawrence Livermore National Laboratory
  - $13.4 M in Computational Partnerships for Co-design

See the Fast Forward talk presented Terri Quinn

# X-Stack II FOA

- ASCR identified research needs through community workshops
  - Exascale Programming Challenges workshop, July 27-29, 2001 at University of Southern California (http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/ProgrammingChallengesWorkshopReport.pdf )
  - Exascale Tools Workshop, October 13-14, 2011 Annapolis, MD (http://science.energy.gov/~/media/ascr/pdf/research/cs/Exascale%20Workshop/Exascale_Tools_Workshop_Report.pdf )
- X-Stack II Funding Opportunity Announcement released November 22, 2011 with Letters of Intent due December 19, 2011 and proposals due February 6, 2012.
  - Available funding up to $15,000,000 per year for three years. Anticipated project funding between $500,000 - $4,000,000 per project.
  - Topic areas: basic research that represents significant advances in programming models, languages, compilers, runtime systems and tools that address fundamental challenges and multiple components (scalability, programmability, portability, resilience and energy efficiency) related to the system software stack for Exascale computing
  - Received 71 Letters of Intent and 68 full proposals
  - 67 proposals reviewed
    - 24 – Lab led
    - 36 – University led
    - 7 – Industry led

# *Other Exascale Activities*

- ASCR and NNSA/ASC Exascale PIs meeting April 19-20, 2012 in Portland Oregon to contribute to the exascale software research plan
  - Articulate key dependencies and crosscutting issues between ASCR and ASC exascale research efforts;
  - Identify key technical/research gaps where further development and investments are needed for the Exascale Software Plan;
  - Contribute input into the development of the Exascale Software Plan;
  - Consider how to engage the co-design projects in the development of the Exascale software stack

- JASON Study – June 27-29, 2012 on the technical challenges associated with developing scientific and national security applications for exascale computing
  - Applications: It is likely that a future exascale platform will utilize a hierarchical memory and network topology. As a result, there may be barriers to optimal performance for certain types of scientific applications.
    - What are the technical issues associated with mapping various types of applications with differing computation and communication platforms to future exascale architectures
    - What are the technical challenges to building hardware that can respond to different application requirements?
  - Programming environments: The development of application codes for future exascale platforms will require the ability to map various computations optimally onto a hierarchical computing fabric. In the past programming tools have been afterthoughts for high performance platforms.
    - What are the challenges in designing such tools that can also be gracefully evolved as the hardware evolves?
  - Economic and national security impacts:
    - What are the economic and national security impacts of failure to execute the DOE ECI?
    - What application capabilities will emerge in the absence of an initiative?

See Mike Heroux's presentation

# *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/