



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# **ASCR Update**

**November 9, 2010**

**Daniel Hitchcock**

**Acting Associate Director**

**Advanced Scientific Computing Research**

# Congressional FY11 Budget Action

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- **Senate:**
  - SC: \$5.012B , \$109.4M under the request
  - ASCR: \$418M, \$8M under the request
- **House:**
  - SC: \$4.9B, \$221.0M under the request, \$4M under the FY 2010 enacted
- **Continuing Resolution at 2010 funding level through December 3<sup>rd</sup>**



# China Wrests Supercomputer Title From U.S.

-- New York Times, October 28, 2010



Tianhe-1A –

- Hybrid architectures composed of Intel and Nvidia chips
- Chinese developed interconnect
- Linpack: 2.5 petaflops



# Staffing

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- **Positions filled**
  - Facilities Division Director: Dan Hitchcock
- **Offers made**
  - Computer Scientist – GS 15
  - Mathematician/Physical Scientist – GS 15
  - Mathematician/Physical Scientist – GS 12
- **Vacancy announcements Closed:**
  - Director, Computational Science and Research Partnerships (SciDAC) Division



# Recognitions



On October 14, 2010, Dr. Warren Washington was named one of ten researchers to receive the **National Medal of Science** for his fundamental contributions to the understanding of Earth's coupled climate system through numerical simulation, leadership in U.S. science policy, and inspiring mentorship of young people of all backgrounds and origins.



# Recognitions: Jim Demmel

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The IEEE named Jim Demmel as the winner of this year's Sidney Fernbach Award, which recognizes outstanding contributions in the application of high performance computing using innovative approaches. Dr. Demmel was recognized “for computational science leadership for creating adaptive, innovative high performance linear algebra software.” The award will be formally presented at the SC10 Conference .



# Recognitions: Alexandre Chorin and James Sethian

**Berkeley Lab's Alexandre Chorin and James Sethian won prestigious prizes from the International Council for Industrial and Applied Mathematics (ICIAM) for groundbreaking work in applied math, with impacts ranging from fluid mechanics and aerodynamics to medical imaging and semiconductor manufacturing.**

**Chorin won the 2011 Lagrange Prize from ICIAM for his groundbreaking work in applied math. A member of the Berkeley Lab Mathematics Group and professor of Mathematics at UC Berkeley, Chorin was honored for "his fundamental and original contributions to applied mathematics, fluid mechanics, statistical mechanics, and turbulence modeling." The Lagrange Prize provides international recognition to mathematicians who have made an exceptional contribution to applied mathematics throughout their career.**



**Sethian, leader of the Berkeley Lab Math Group, won the 2011 Pioneer Prize from ICIAM. Sethian, who is also a professor of mathematics at UC Berkeley, was honored "for his fundamental methods and algorithms that have had a large impact in imaging and shape recovery in medicine, geophysics and tomography, and drop dynamics in inkjets." The Pioneer Prize recognizes pioneering work introducing applied mathematical methods and scientific computing techniques to an industrial problem area or a new scientific field.**



# Novel mathematical approach to modeling and simulation of plasma confinement

## Challenge:

- Heat transport in magnetized plasmas is a problem of fundamental interest in controlled fusion, space plasmas, and astrophysics research.
- Simulating extreme transport anisotropy: parallel transport to perpendicular transport

## Accomplishments:

ORNL researchers have developed a novel approach that enables the **scalable, accurate and efficient computation** of parallel transport in **general magnetic fields** with local or nonlocal closures.

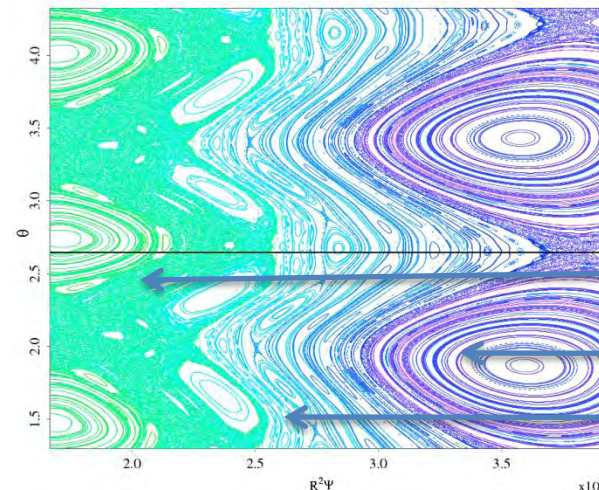
- Scalable, fully implicit Newton-Krylov Multigrid solver for extended MHD
- Novel asymptotic-preserving formulation for the anisotropic transport equation

**Contacts:** Luis Chacon and Diego del-Castillo-Negrete, ORNL

## First-ever simulation of:

- The *fractal structure* of the temperature profile in a weakly chaotic field (shown on the right)
- Effective radial transport due to *non-local parallel transport* in fully chaotic magnetic fields.

## Poincare plot of a chaotic magnetic field



*In the presence of perturbations, the magnetic field topology in confined fusion plasmas exhibits a **fractal mixture** of:*

**Chaotic orbits**

**Islands**

**Barriers**



# Automatic Performance Tuning (Auto-tuning)

Samuel Williams, Leonid Oliker, James Demmel, Kamesh Madduri, plus many others (LBNL)

## ASCR- Computer Science Highlight

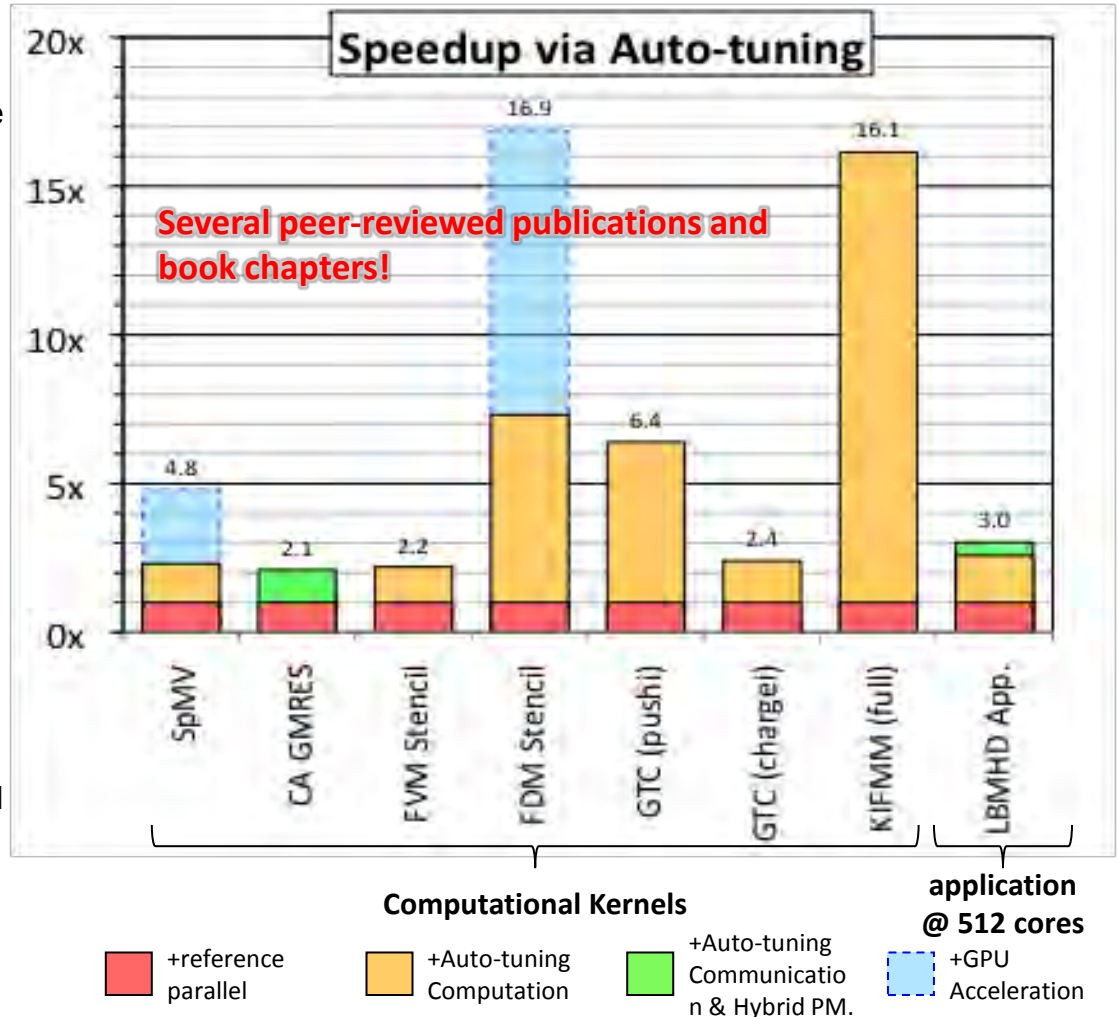
Accomplishments FY2010

### Objectives

- Develop optimizations for emerging hardware
- Create code generators that productively produce code for all variations of viable optimizations
- Perform efficient search of the very large and high-dimensional optimization space of automatic performance tuning

### Impact

- **Enabled optimizations of computational kernels and applications by auto-tuning:**
  - Code transformations (loop tiling, unroll-and-jam ~ ATLAS, FFTW )
  - alternate data structures (e.g. register blocking for sparse matrices ~ OSKI)
  - parallelization (multicore-aware, hybrid models, problem decomposition, synchronization, GPU acceleration)
  - algorithmic parameters (k-steps in Krylov subspace methods, particles per box in Fast Multipole Method, shape of multigrid V-cycle)



# ARRA Update

## ASCR's Recovery Act Projects (\$153.9M)

- Leadership Computing Facility Upgrades (\$19.9M) Six-core upgrade to Oak Ridge LCF machine to take the OLCF to ~2 Petaflops peak
  - **--- COMPLETED**
- Advanced Networking Initiative (\$66.8M) 100Gbps optical networking testbed and tools
  - **Selected research topics projects through Funding Opportunity Announcement and paperwork for awards in Chicago**
- Advanced Computer Architectures (\$5.2M) Research on next generation technologies
  - **Reviewers of Progress reports found that projects were on track and making satisfactory progress**
- Magellan (\$32.8M) Research to demonstrate viability of cloud computing for mid-range computational science
  - **“MG-Rast” code did metagenomics analysis across both sites**
  - **Programmatic review of progress completed**
  - **Implemented methods for securing private clouds**
  - **Benchmarking and analyzing application performance in cloud environments**
  - **Evaluating various open source cloud software stacks (Eucalyptus, Nimbus, OpenStack)**
  - **Collecting workload characteristics for DOE applications**
- SciDAC-e (\$29.2M) Supplement and leverage existing SciDAC investments to advance the high performance computational capabilities of the BES - Energy Frontier Research Centers



# ARRA Update: SciDAC-e

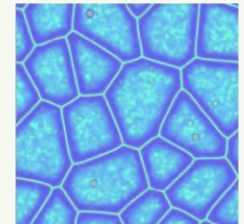
*ARRA Second year, 4<sup>th</sup> Quarter Milestone: “Charge ASCAC, in coordination with Basic Energy Sciences, to convene an expert panel to review SciDAC-e activities”*

***Milestone will not be met. SciDAC-e awards (engagements with EFRCs) were made late in FY2010. No results will be available for review this CY.***

***ACTION PLAN: Charge ASCAC in March, 2011 to organize a joint review of SciDAC-e with BESAC and provide a report August, 2011.***

## **Progress since August 2010:**

- Supplemental awards to SciDAC Centers and Institutes to support BES EFRCs to develop a high-performance computing capability relevant to the goals of the EFRC
  - 14 projects awarded in FY2010; funds arrived at the end of August
  - Start-up activities: postdocs hired at TOPS (1), VACET (1)
- Applied Math projects: research ongoing
- Postdocs at ALCF, OLCF, and NERSC
  - 6 PDs on board at NERSC (goal: 8 PDs)
  - 6 PDs on board at OLCF (goal: 10 PDs)
  - 7 PDs on board at ALCF (goal: 10 PDs)



# ASCR Exascale Research Kick-off Meeting

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- **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
- **Tentative dates: March 7-11, 2011**



# Early Career Research Program (FY11) - ECRP

FY11 – 2<sup>nd</sup> year of competition:

- Solicitation issued - July 1
- Pre-applications due - Aug 13
- Encourage applications – Sep 14
- Full applications due Nov 9

Schedule for 2011:

- ASCR Panel Reviews, Jan 11-13
  - Applied Mathematics
  - Computer Science
  - Computational Science / Biology
  - Networking

**About ECRP**  
ASCR, 22 October 2010 (created 19 October 2010)  
The purpose of this Early Career Research Program is to support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by the DOE Office of Science. In 2011, up to \$15 million in funding will be awarded to support at least 50 early career researchers for five years at U.S. academic institutions and DOE national laboratories. University awards will be at least \$150,000 per year for five years and are intended to provide research expenses and summer salary over and above the awardee's academic-year faculty salary. For DOE national laboratories — where DOE funding typically covers a researcher's full year-round salary — the award will be at least \$500,000 per year for five years to provide equivalent support.

This is the second year of an annual competition. To be eligible for the competition, a researcher must be an untenured, tenure-track assistant or associate professor at a U.S. academic institution or a full-time employee at a DOE national laboratory. The applicant must also have received a Ph.D. within the past ten years.

Opportunities exist in the following six program areas: Advanced Scientific Computing Research (ASCR); Biological and Environmental Research (BER); Basic Energy Sciences (BES), Fusion Energy Sciences (FES); High Energy Physics (HEP), and Nuclear Physics (NP).

DOE Office of Science ECRP [website](#) - official website for the program  
Early Career Research Program for FY11 - [announcement](#)  
Early Career Research Program - ASCR [webpage](#)

**Panel Review**  
ASCR, 24 October 2010 (created 19 October 2010)  
Schedule for panel review at Hyatt Regency Bethesda - Jan 11-13, 2011

Panels/Dates	Tues, Jan 11	Wed, Jan 12	Thurs, Jan 13
Panel Room 1	Applied Math	Applied Math	Applied Math
Panel Room 2	Computer Science	Computer Science	Computational Applications
Panel Room 3	Computational Science*	Applied Math	Networking*
Panel Room 4	open	open	open

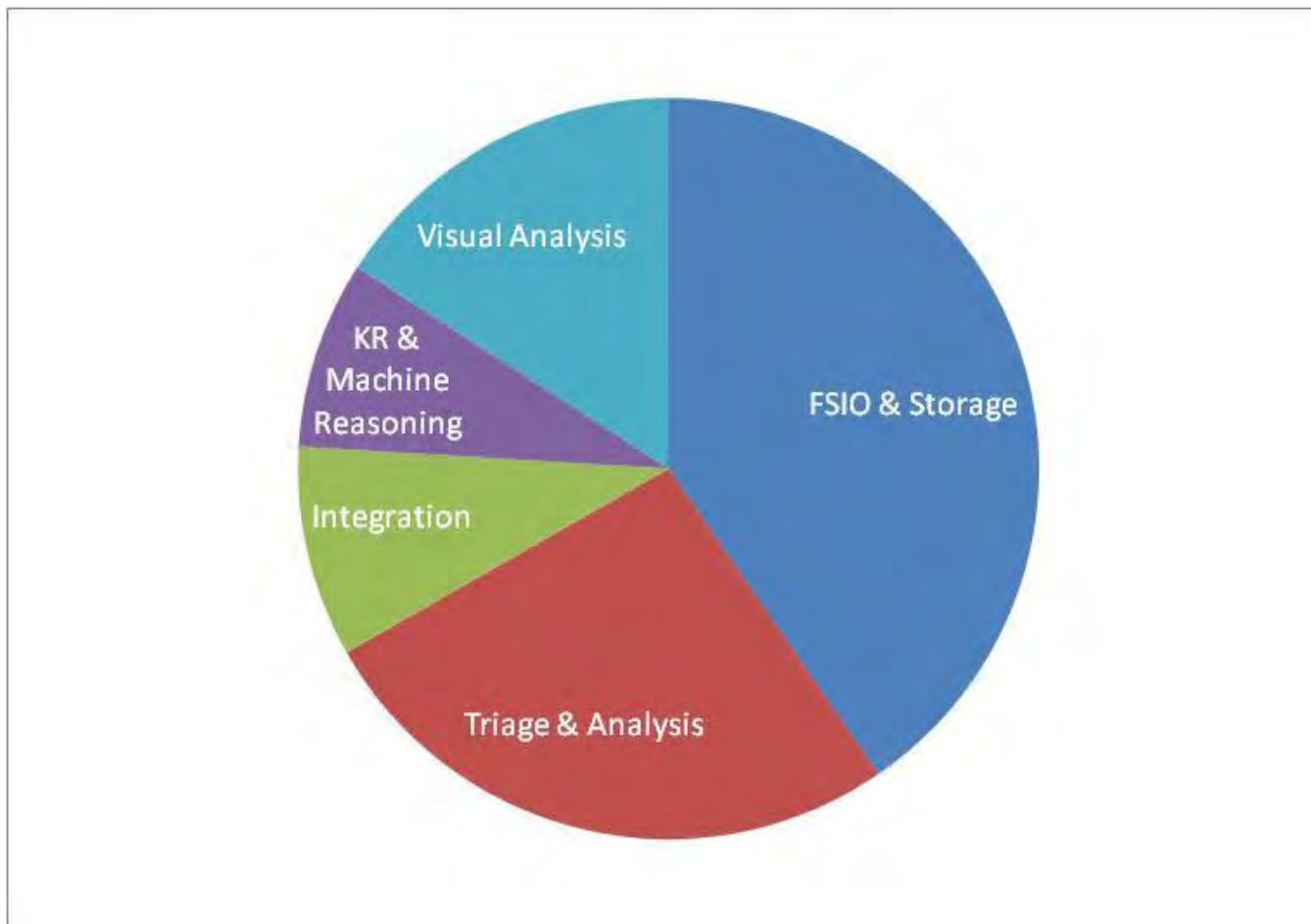
Program areas - color key: Applied Math; Computer Science; Computational Science; Networking;  
Computational Applications  
\*\* = confirmed panel room and date





# Scientific Data Management & Analysis

FOA (37 proposals requesting \$22M/year; 11 projects funded at ~\$5M/year)



60 % Lab

40% University and Industry





# Sci. Data Mgmt. & Analysis at Extreme Scale

(37 proposals requesting ~\$22/yr)

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- **Dynamic Non-Hierarchical File Systems for Exascale Storage**
  - University of California, Santa Cruz
- **Runtime System for I/O Staging in Support of In-Situ Processing of Extreme Scale Data**
  - Oak Ridge National Laboratory; Lawrence Berkeley National Laboratory; Georgia Institute of Technology
- **Bringing Exascale I/O Within Science's Reach: Middleware for Enabling & Simplifying Scientific Access to Extreme Scale Data**
  - Lawrence Berkeley National Laboratory; Pacific Northwest National Laboratory
- **Adding Data Management Services to Parallel File Systems**
  - University of California, Santa Cruz; Lawrence Livermore National Laboratory
- **Scalable and Power Efficient Data Analytics for Hybrid Exascale Systems**
  - Northwestern University; Lawrence Berkeley National Laboratory; Oak Ridge National Laboratory



# Sci. Data Mgmt. & Analysis at Extreme Scale

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- **A Pervasive Parallel Processing Framework for Data Visualization & Analysis at Extreme Scale**
  - Sandia National Laboratories; Kitware, Inc.; University of California, Davis
- **An Information-Theoretic Framework for Enabling Extreme-Scale Science Discovery**
  - Ohio State University; New York Institute of Technology; Argonne National Laboratory
- **Enabling Scientific Discovery in Exascale Simulations**
  - Lawrence Livermore National Laboratory; University of Minnesota
- **Graph-Based 3D Flow Field Visual Analysis**
  - Pacific Northwest National Laboratory
- **Topology-Based Visualization & Analysis of Multidimensional Data & Time-Varying Data at the Extreme Scale**
  - Lawrence Berkeley National Laboratory

**Ten projects funded at ~\$5M/yr**



# SciDAC Recompetition Planning

- **DOE SciDAC program manager working group reconstituted**
  - Representation from all Office of Science programs and the NNSA
  - Activities: planning, 'lessons learned' and 'gap' analysis
- **Strategy and Schedule**
  - **January-February, 2011: Issue Funding Opportunity Announcement for SciDAC Institutes**
    - Coordinated investments in applied math, computer science, algorithms, code development, data analytics, visualization, software development and outreach aligned with SciDAC goals and cross-cutting strategic needs identified by ASCR's SciDAC funding partners.
    - ASCR funded
    - Anticipated award date- late FY2011
  - **Spring-Summer, 2011: Issue the first in a series of focused FOAs for domain science components of SciDAC**
    - Jointly issued and funded by ASCR with one, or more, SC program offices and/or the NNSA
    - Requesting proposals that address topics of strategic importance to the domain science funding office(s) and ASCR.
    - Tangible links to the SciDAC Institutes
    - Anticipated award date- early FY2012



# Phase Change in Computing

