U.S. DEPARTMENT OF ENERGY | Office of Science

SciDAC: the *next* generation

2012 SciDAC PI Meeting
10 September 2012

Dr. Daniel Hitchcock
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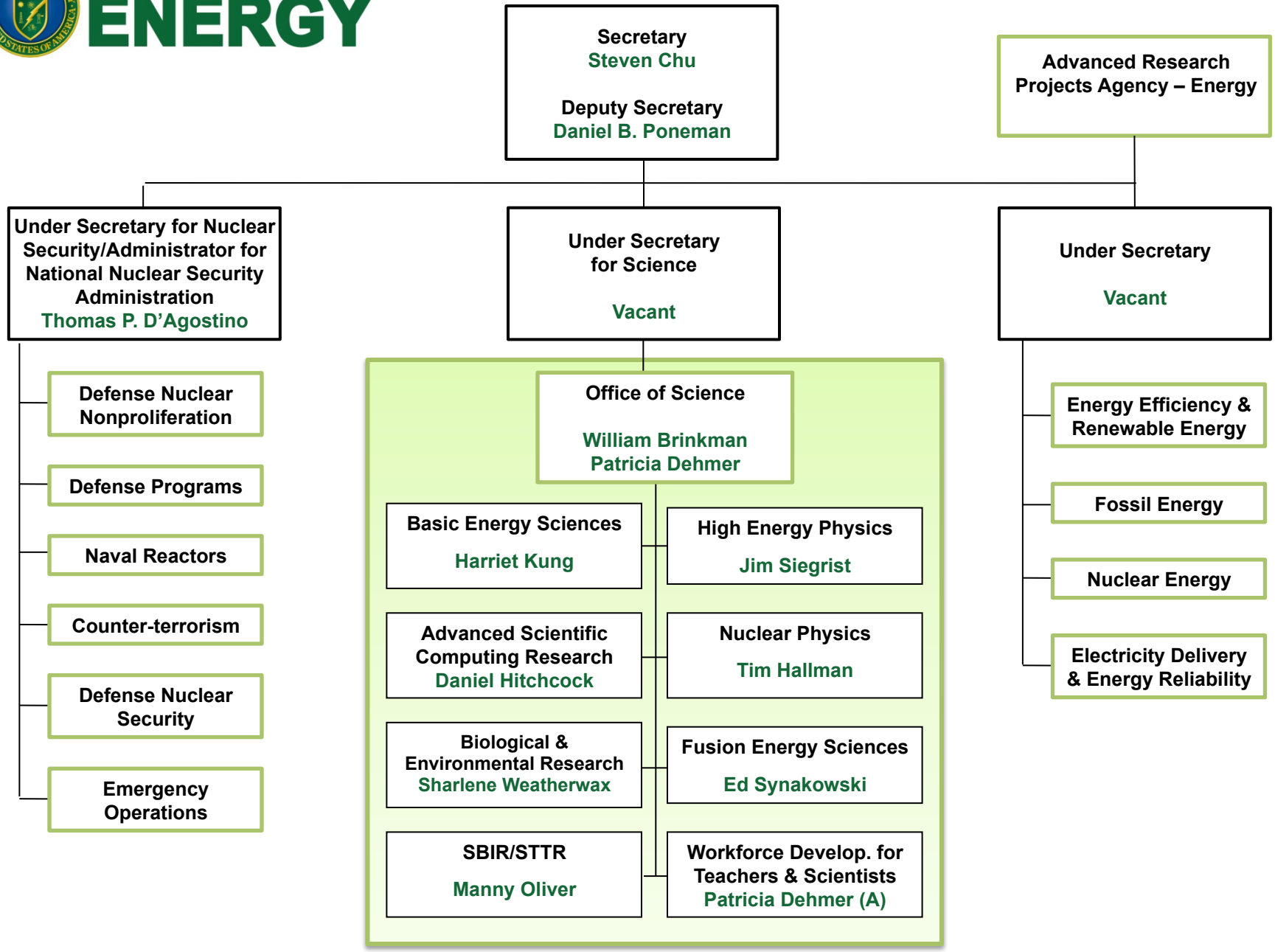
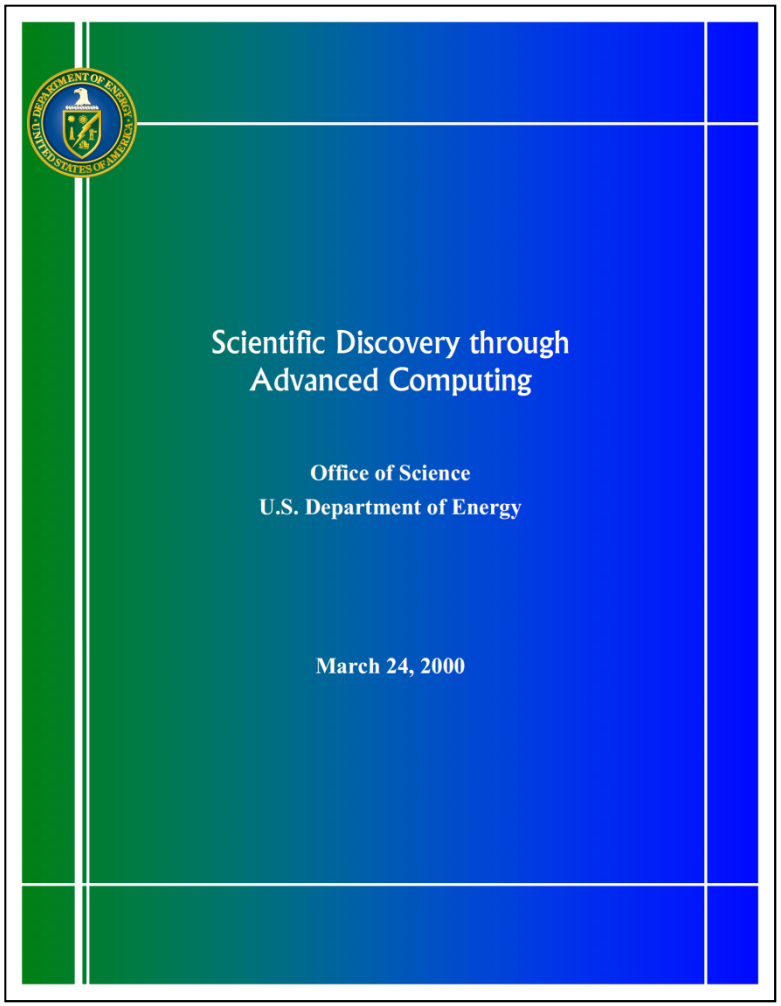
Office of Science, U.S. Department of Energy

U.S. DEPARTMENT OF ENERGY



And then there was SciDAC



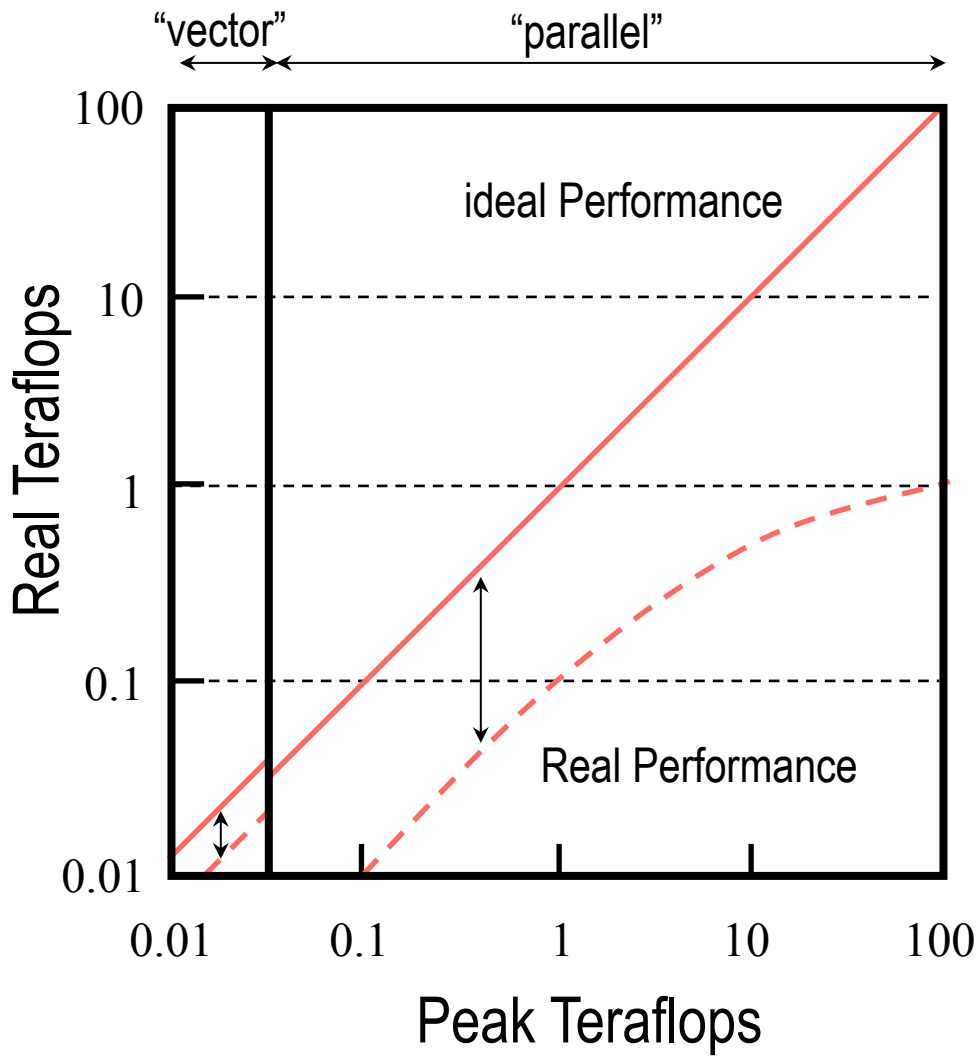
On March 30, 2000, SC submitted a plan for scientific computing to the EWD Subcommittees of the Appropriations Committees of the U.S. Congress.

The plan, “Scientific Discovery through Advanced Computing,” outlined a five-year program to develop the *Scientific Computing Software* and *Hardware Infrastructure* needed to use **terascale** computers to advance research programs in basic energy sciences, biological and environmental research, fusion energy sciences, and high energy and nuclear physics.

SciDAC Goals (2001)

- **Create scientific codes** that take advantage of terascale computers.
- Create mathematical and computing systems software to efficiently use terascale computers.
- Create a collaboratory environment to enable geographically separated researchers to work together and to facilitate remote access to facilities and data.

The Software Challenge

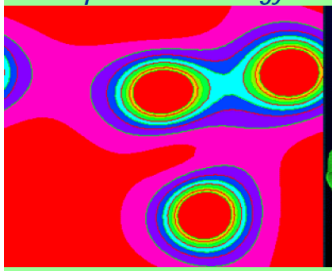


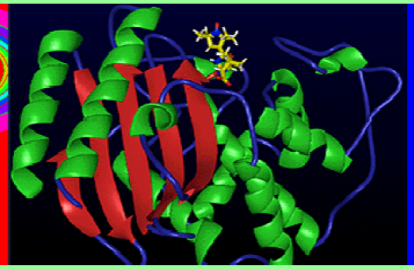
On "vector" machines, scientific codes realized 40-50% of peak performance

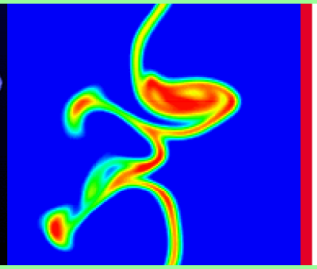
On "parallel" machines, existing scientific codes realize as little as 5-10% of peak performance

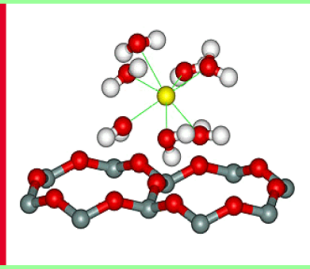
Scientific Discovery Through Advanced Computing

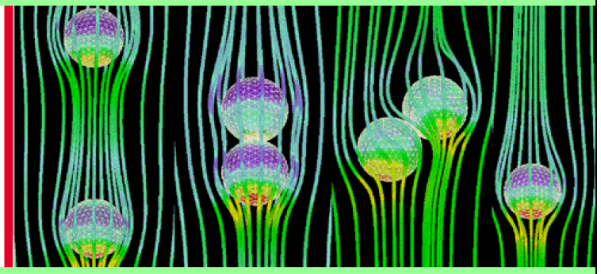
U.S. Department of Energy *Office of Science*

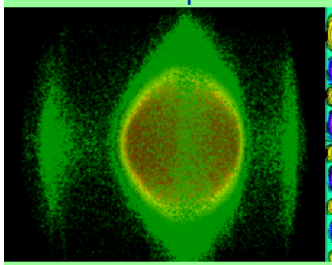

Vortices in a superfluid

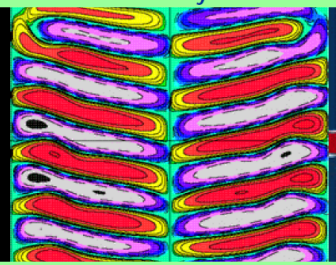

Protein dynamics


Turbulent methane flame

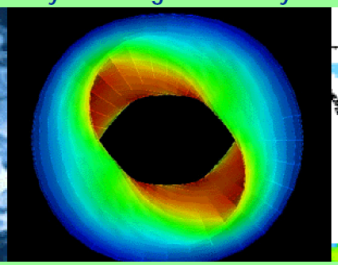

Clay-mineral geochemistry

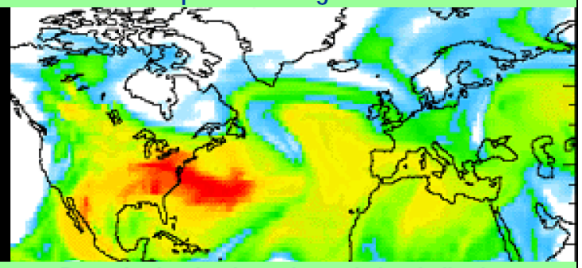

Two spheres mixing in a stream

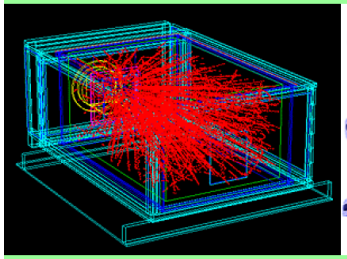

HEP particle beam halo

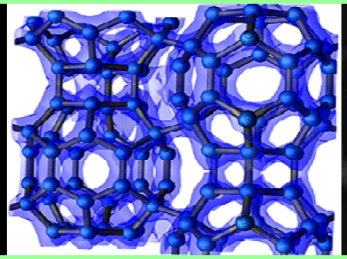

Transport barrier dynamics

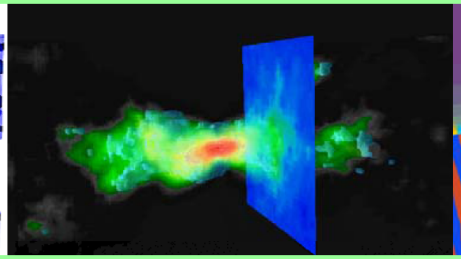
Combustion turbulence modeling

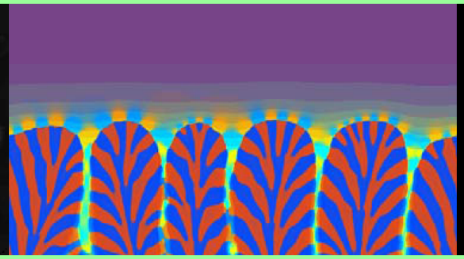

Fusion magnetic field

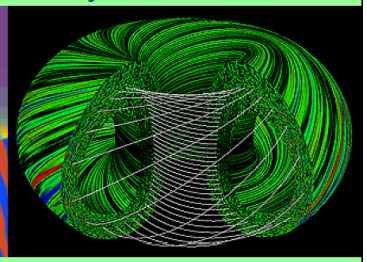

Perturbation in clear-sky and cloud albedo

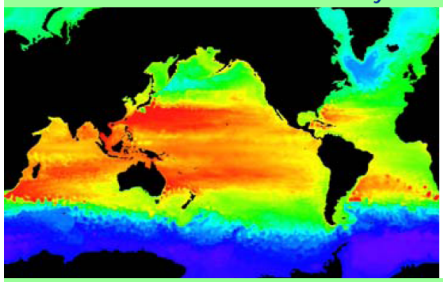

Au-Au collision

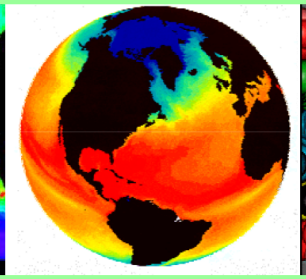

Crystal structure for C_{36} solid

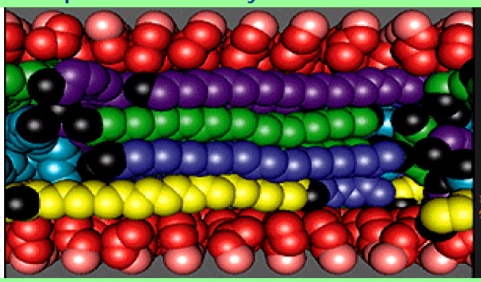

Lattice quantum chromodynamics

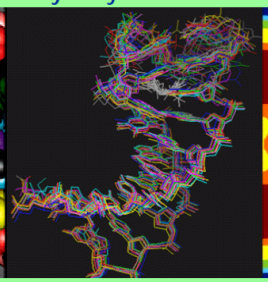

Binary alloy solidification

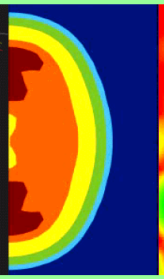

Perturbed plasma density

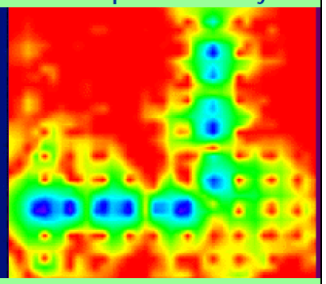

DOE Parallel Climate Model


Sea surface temperature

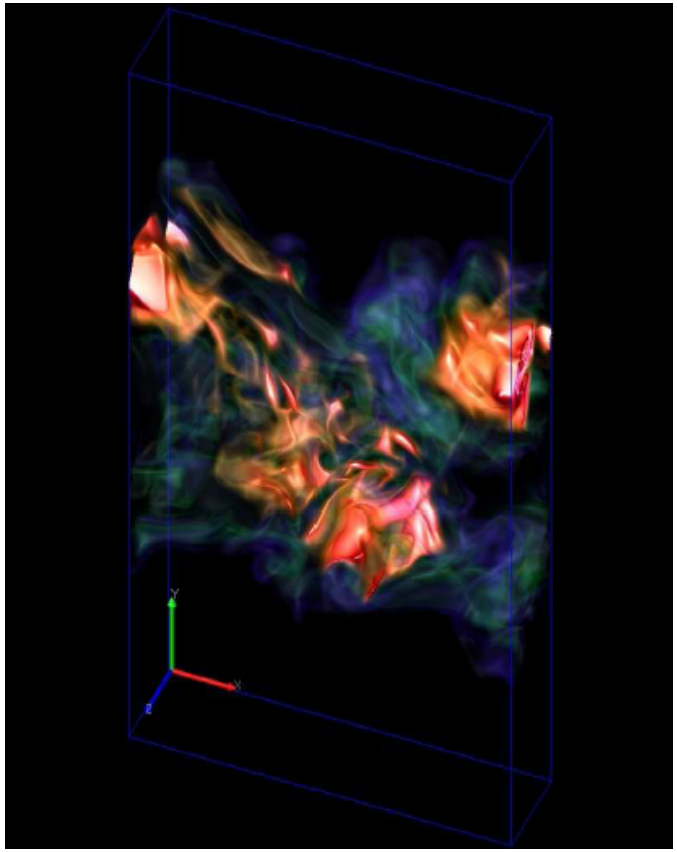

Molecular simulation of complex fluids


Structural biology


Nuclear theory


Waveguide optics

SciDAC-1 Successes



Hydroxyl radical in a turbulent jet flame

- SciDAC teams created first laboratory-scale flame simulation in three dimensions to better understand combustion which provides 80% of the energy used in the U.S.
- Magnetic fusion scientists and applied mathematicians simulated techniques for re-fueling fusion reactors
- Teams developed new methods for simulating improvements in future particle accelerators
- Partnerships improved effectiveness of scientific applications codes between 275% to over 10,000%
- The SciDAC data mining tool Sapphire awarded a 2006 R&D100 award

SciDAC-1 → SciDAC-2

The SciDAC program was re-competed in FY2006

Goals:

- Create comprehensive, scientific computing software infrastructure to enable scientific discovery in the physical, biological, and environmental sciences at the petascale
- Develop a new generation of data management and knowledge discovery tools for large data sets (obtained from scientific user facilities and simulations)
- >230 proposals received requesting approximately $1 B

SciDAC-2 (2006)

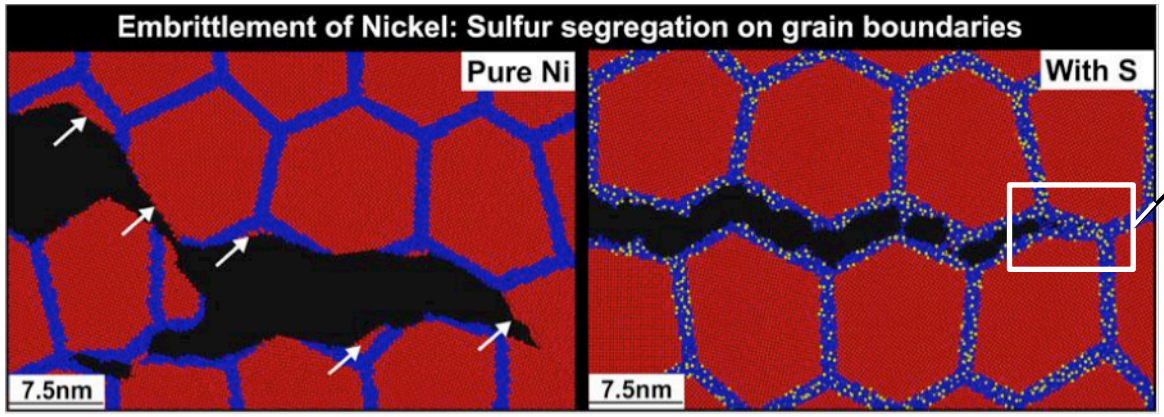
Computational Collaborations to Drive Scientific Discovery

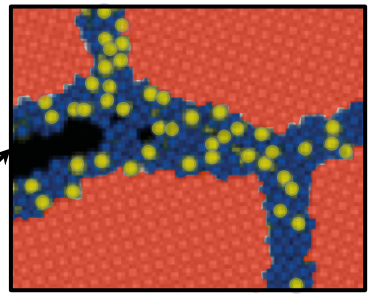
One FOA to rule them all, One FOA to find them,
One FOA to bring them all and in the darkness bind them

- **31 Projects**
  - 9 Centers
  - 4 Institutes
  - 18 Projects in application areas
    - *Astrophysics, Climate, Biology, Fusion, Petabytes, Materials & Chemistry, Nuclear physics, High Energy physics, QCD, Turbulence, Groundwater*
  - 1 SciDAC Outreach Center

Stress Corrosion Cracking

Molecular Dynamics Simulation Reveals Mechanisms of Nickel Fracture





Fracture simulations for nanocrystalline nickel without and with amorphous sulfide grain-boundary phases, showing ductile, transgranular tearing and brittle, intergranular cleavage.

- The performance and lifetime of materials used in nuclear technology and in advanced power generation are severely limited by corrosive environments and extreme conditions.
- Premature failure of materials can result from undetected stress corrosion cracking.
- Annually, corrosion costs about 3% of the U.S. gross domestic product.
- 48-million-atom simulation on Argonne Leadership Computing Facility showed a link between sulfur impurities segregated at grain boundaries of nickel and embrittlement. An order-of-magnitude reduction in grain-boundary shear strength, combined with tensile-strength reduction, allows the crack tip to always find an easy propagation path in this configuration. This mechanism explains an experimentally observed crossover from microscopic fracture to macroscopic cracks due to sulfur impurities.
- P. Vashishta (USC)

An improved solution framework for Greenland Ice Sheet simulation – K. Evans, ORNL

Objectives

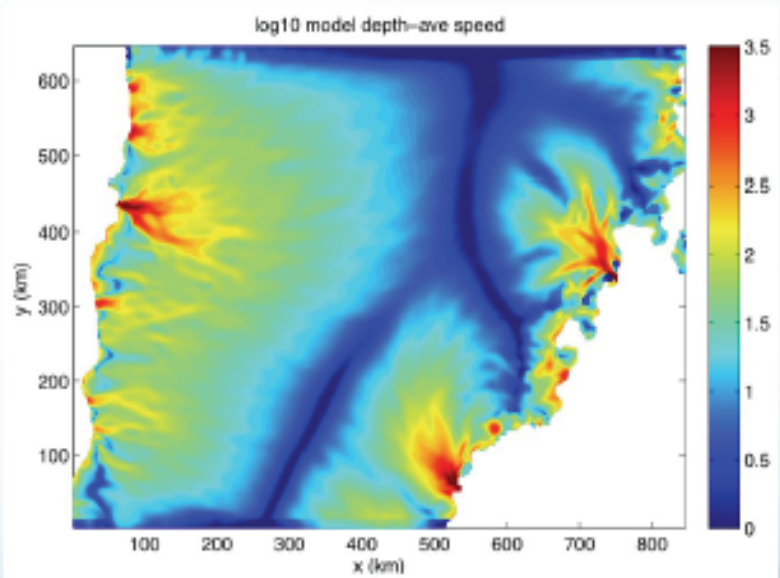
Provide a state-of-the-art ice sheet model with continuous access by the climate community

Implement parallel, scalable capability to allow efficient high-resolution simulations

Design to allow ongoing code extensions by ice sheet modelers

Impact

Continental ice sheet models are currently the frontier of global climate modeling, as they are just now being coupled to global Earth system models.



Courtesy S. Price, LANL, presented at AGU Nat'l meeting, Dec. 2010

Progress

- Range of test cases and boundary conditions to span problem space
- Tuned, steady-state simulation using higher-order velocity solver
- Suites of high resolution (<5km) steady state runs desired to explore parameter space
- Eventually, time evolving ice sheet runs coupled with the ocean to provide predictive capability

SciDAC-2 → SciDAC-3 (2011)

Specific goals and objectives for the SciDAC Institutes:

- Tools and resources for lowering the barriers to effectively use state-of-the-art computational systems;
- Procedures for taking on computational grand challenges across different science application areas;
- Procedures 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
- Letters of Intent (LOI), not required, are strongly encouraged - March 30, 2011
- Proposal due date – May 2, 2011
- FY11 Awards for 3 SciDAC Institutes completed – July 2011

○ Solicitation for Scientific Data Management, Analysis & Visualization

✓ FY12 - Posted Sep 16; LOIs due Oct 12; Proposals due Nov 9; Awarded in Feb 2012

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

FASTMath Director – Lori Diachin Scalable solvers & discretizations	QUEST Director – Habib Najm Uncertainty Quantification	SDAV Director – Arie Shoshani Scalable data management, analysis & visualization	SUPER Director – Robert Lucas Performance tools & code optimization
Lawrence Livermore (CA)	**Sandia (CA)**	**Lawrence Berkeley (CA)**	**Univ of Southern CA**
Argonne (IL)	Los Alamos (NM)	Argonne (IL)	Argonne (IL)
Lawrence Berkeley (CA)	Duke University (NC)	Lawrence Livermore (CA)	Lawrence Berkeley (CA)
Sandia (CA & NM)	MIT (MA)	Los Alamos (NM)	Lawrence Livermore (CA)
RPI (NY)	Univ of Southern CA	Oak Ridge (TN)	Oak Ridge (TN)
	Univ of Texas, Austin (TX)	Sandia (NM)	Univ of CA, San Diego (CA)
		Univ of CA, Davis (CA)	Univ of Maryland (MD)
		Georgia Tech (GA)	Univ of North Carolina (NC)
		North Carolina St Univ (NC)	Univ of Oregon (OR)
		Northwestern (IL)	Univ of Tenn, Knoxville (TN)
		Ohio State Univ (OH)	Univ of Utah (UT)
		Rutgers Univ (NJ)	
		Univ of Utah (UT)	
		Kitware, Inc (NY)	

FASTMath - Frameworks, Algorithms & Scalable Technologies for Mathematics
QUEST - Quantification of Uncertainty in Extreme-Scale Computations
SDAV - Scalable Data Management, Analysis & Visualization
SUPER - Institute for Sustained Performance, Energy & Resilience

Lead
National Labs
Universities
Industry

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Strategic ASCR – SC Program Partnerships

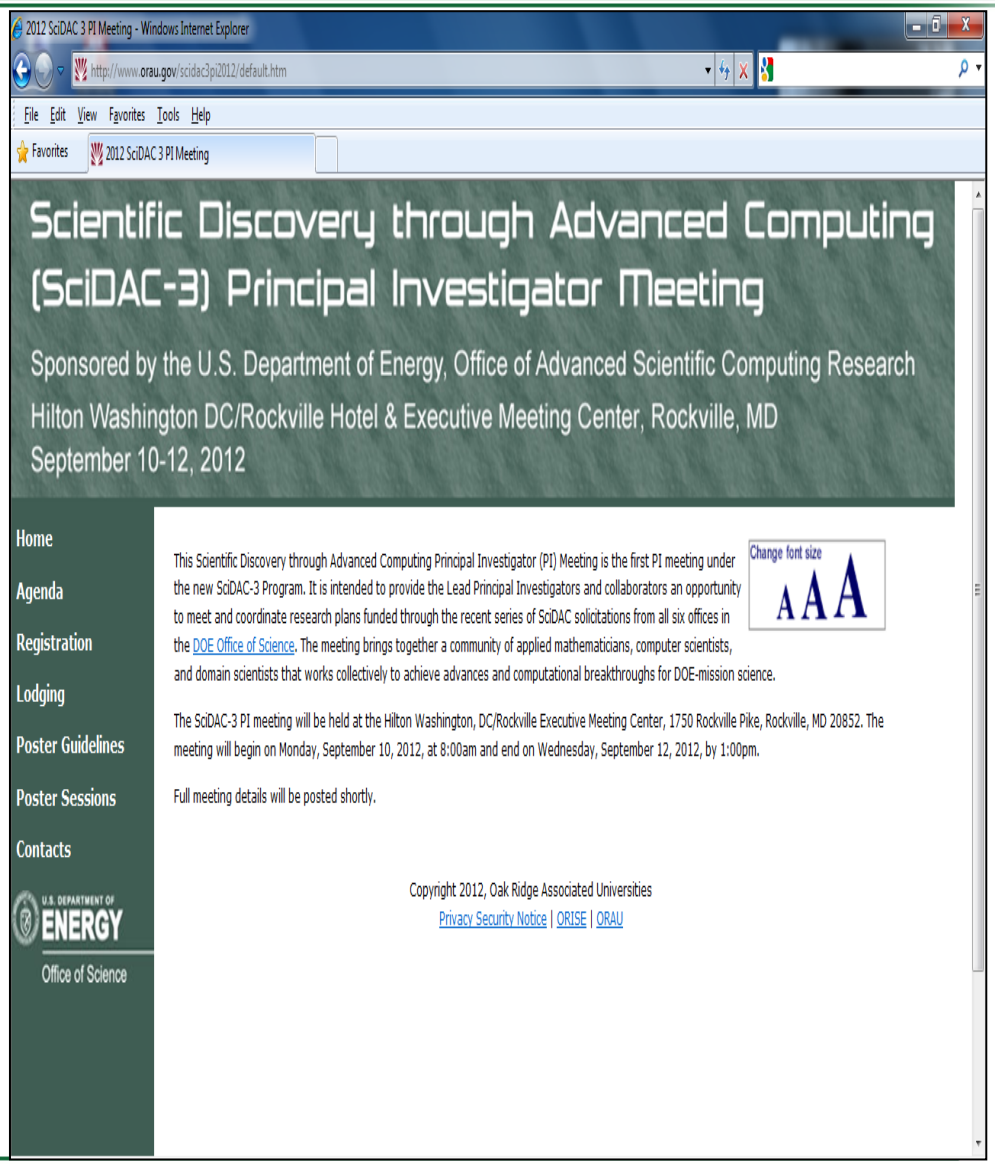
- **Goals and Objectives**
  - Partner with SC Programs to combine domain science expertise with the best applied mathematics and computer science in order to enable advances in program missions of strategic importance

- **Criteria for successful Partnerships**
  - 1. Exploit leadership class computing resources to advance scientific frontiers in an area of strategic importance to the Office of Science
  - 2. Effectively link to the intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools at one, or more, SciDAC Institutes
  - "Reviewers…will be asked to comment upon the feasibility, benefits, and management of the proposed collaborations between the [*domain scientists*] supported by [*the SC Program*] on the one hand, and the computational scientists (i.e., applied mathematicians and computer scientists/engineers) supported by ASCR on the other."

Five SciDAC Joint FOAs published

August 3 – September 22, 2011

FOA/ LAB	Partner Program	Partner PM	ASCR PM	Topics	Max. ($1,000)	Projects	Duration (Years)
11-571	FES	John Mandrekas	RL	Fusion Plasma Science	$33,000	1-4	5
11-580	HEP	Lali Chatterjee	RL	High Energy Physics	$12,000		3
11-581	NP	Ted Barnes	RL	Nuclear Physics	$20,000	1-4	5
11-588	BER	Dorothy Koch	RL	Earth System	$32,500	2-5	5
11-593	BES	Jim Davenport, Mark Pederson	CS	Chemistry, Materials	$30,000	5-12	5

SciDAC-3 Program

- **The Future:**
  - Energy and power aware
  - Massive concurrency
  - Lessons from Codesign and Exascale
- **Broadening Impact**
  - Partnerships with Programs
  - Outreach to Applied Programs
  - Interfaces to Industry