Summary of SciDAC meeting

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SCA Meeting

July 22, 2011

SLAC NATIONAL ACCELERATOR LABORATORY

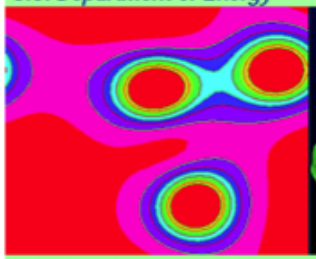
What is SciDAC?

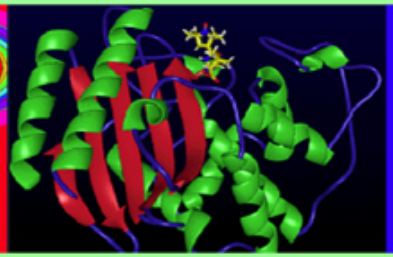
- SciDAC is a DOE funded program lead by the Office of Advanced Scientific Computing Research (ASCR)
- **Sci**entific **D**iscovery through **A**dvanced **C**omputing
    - The program funds Math and CS institutes and centers
    - Funds development science codes in partnership with other offices with the Office of Science, within DOE (NNSA), and with NSF
    - In HEP-four programs:
        - OSG (NP, NSF)
        - Lattice QCD (NP)
        - Accelerator Modeling (NP, BES) < SLAC >
        - Supernova simulations (NP, NNSA) <SLAC>
- Some of ASCR's other portfolio includes ESNET, NERSC, the leadership class facilities at ORNL and ANL
- The SciDAC meeting started as a PI meeting; morphed into a unique meeting
    - The breath makes the meeting impossible to summarize
    - Much of the utility is in private conversations during the poster sessions
    - And this was the very last SciDAC meeting

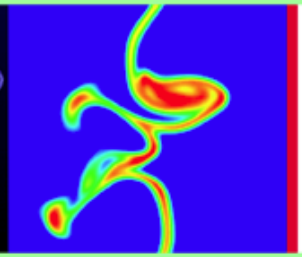
SciDAC 2011 agenda

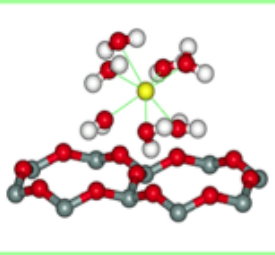
Scientific Discovery Through Advanced Computing

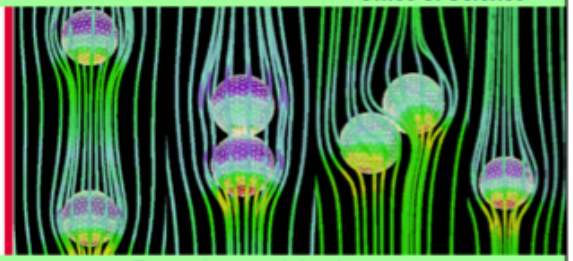
U.S. Department of Energy — *Office of Science*

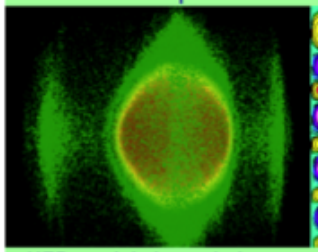

Vortices in a superfluid

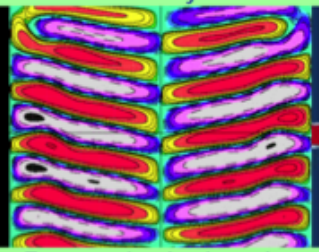

Protein dynamics


Turbulent methane flame

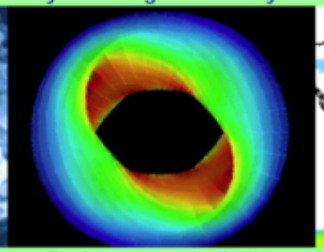

Clay-mineral geochemistry

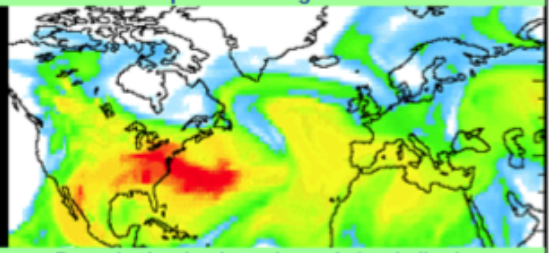

Two spheres mixing in a stream

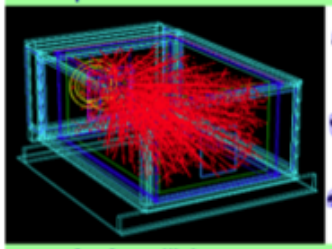

HEP particle beam halo

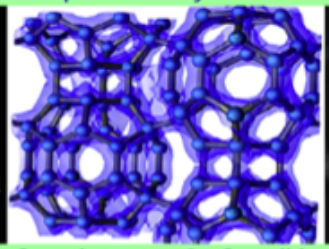

Transport barrier dynamics

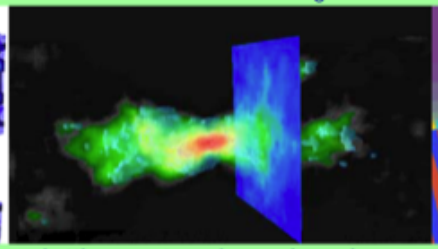

Combustion turbulence modeling

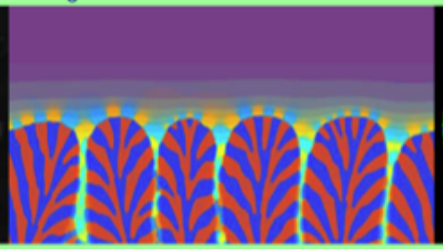

Fusion magnetic field

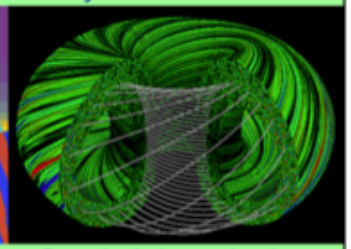

Perturbation in clear-sky and cloud albedo

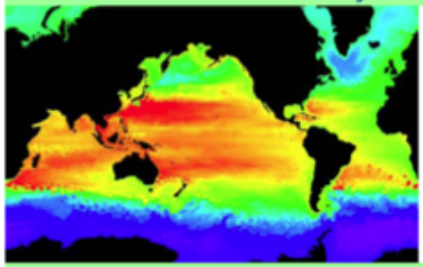

Au-Au collision

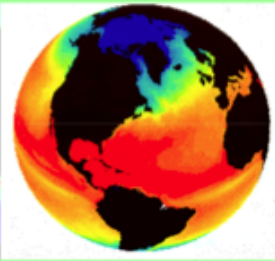

Crystal structure for C_{36} solid

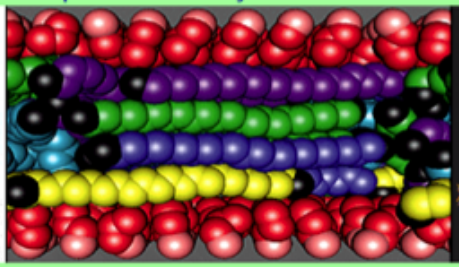

Lattice quantum chromodynamics

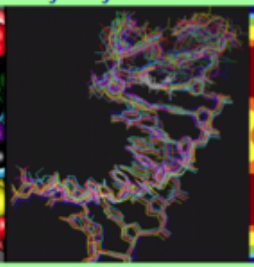

Binary alloy solidification

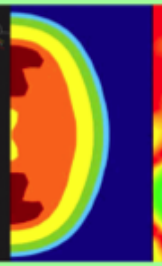

Perturbed plasma density

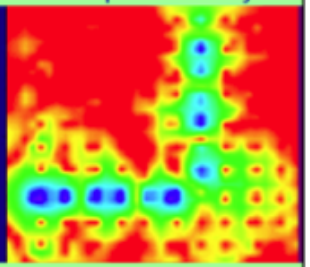

DOE Parallel Climate Model


Sea surface temperature


Molecular simulation of complex fluids


Structural biology


Nuclear theory


Waveguide optics

Impressions

- A stroll through the SciDAC 2011 Agenda
- Because the Institute competition is in process and the FOAs (Funding Opportunity Announce) are expected in August, this conference much less science in the plenary sessions than in the past.
  - The technical talks were very technical
  - More vendor talks than usual
  - Panel discussions were introduced
    - The climate talk was especially interesting
- Fewer non ASCR program managers attended than in the past.

Discussions

- I talked with people about:
  - Accelerator modeling for SciDAC III *
  - Possible collaborative data management projects *
  - Type Ia supernova simulations
  - Computational Cosmology *
  - Performance improvements for G4 *
  - Schemes for federating resources
  - Globus Online
  - The Magellan Cloud project (built with ARRA funds)
  - Mulling/fretting/discussing the single minded focus on exascale

Discussions continue to prepare for proposals with SLAC involvement in some areas.

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SciDAC-1

- 10 year program-Pat Dehmer gave a retrospective
  - Fascinating to learn what motivated the program, how it became broad and how it became to be so tightly linked to the leadership class facilities
- SciDAC I Goals (2001-2006)
  - **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.**

OFFICE OF SCIENCE
FY 2002 PRESIDENT'S BUDGET REQUEST TO CONGRESS
(B/A in thousands of dollars)

	FY 2000 Comparable Approp.	FY 2001 Comparable Approp.	FY 2002 Pres. Request
Science			
Advanced Scientific Computing Research	122,338	165,750	165,750 *

SciDAC II

- The SciDAC program was re-competed in FY2006Goals:
  - 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

(and that was all that was said about SciDAC II)

SciDAC III

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**

Awards- FOA's in development with other SC Offices

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

Expected outcome- New Science.

Timeline

- **Solicitations opened- August 2011**
- **First awards- mid FY2012**

Institutes being awarded now
$13M/year

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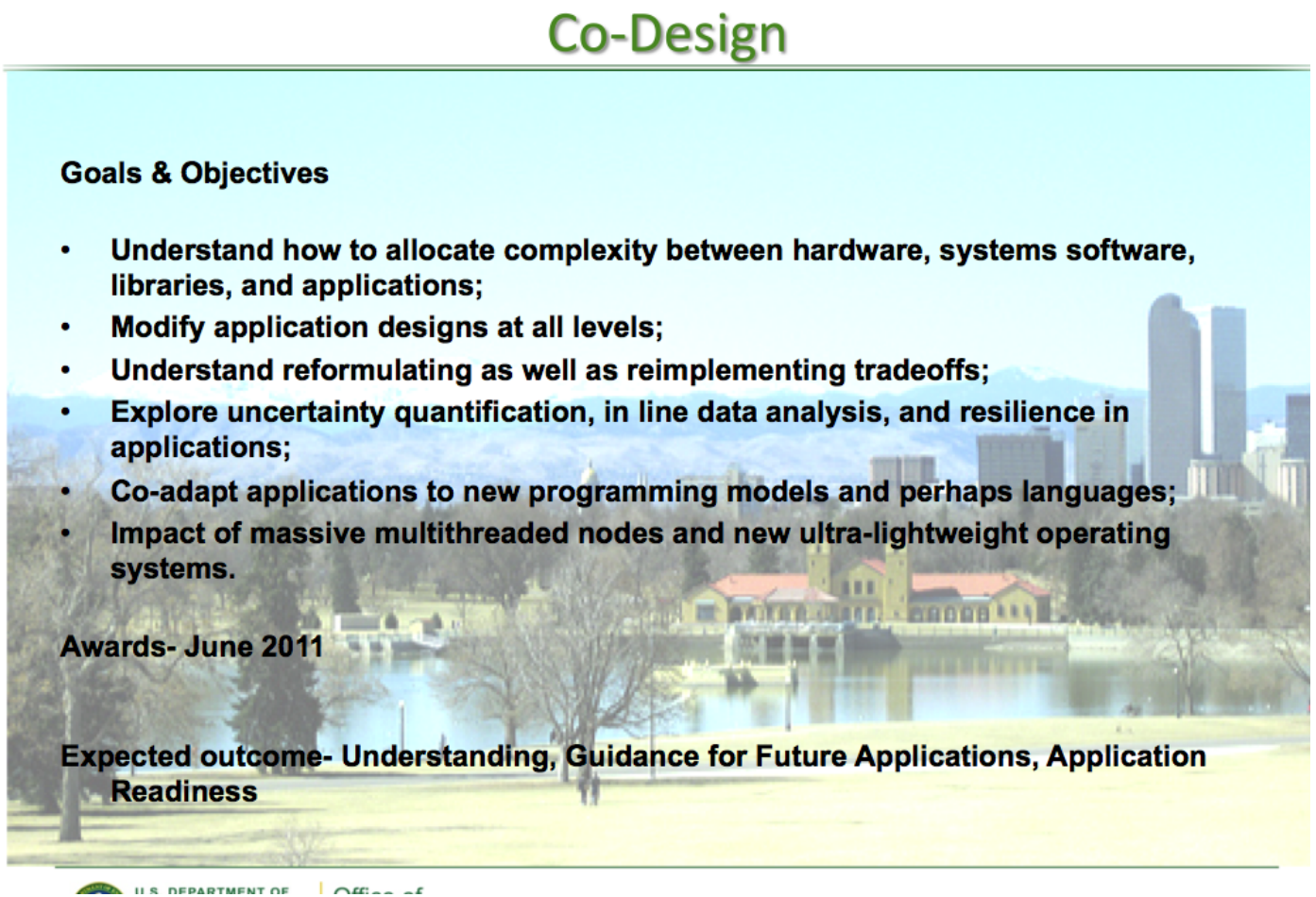
CoDesign



Three awarded

Materials
Reactor Simulations
Combustion