

# U.S. Department of Energy's Office of Science

**Advanced Scientific Computing Research Program** 

## Scientific Discovery through Advanced Computing

-- Status Report --

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307-903-5935

ASCAC Meeting: March 15-16, 2006



## SciDAC Lessons Learned -- Since FY 2001 --

- Computational partnership model works and delivers new science
- Partnerships require ongoing collaboration between program managers in ASCR and other Offices in SC after awards are made
- Intellectual property needs to be considered distributed software efforts
- Sustainability of SciDAC software is an issue



## SciDAC Future...

**Advanced Scientific Computing Research Program** 

### ... as viewed in 2001!

- Initial focus is software
- Priorities in FY 2002 and Beyond are likely to be
  - As SciDAC Teams mature, more demands will be placed on computing and network infrastructure
  - New Scientific Application Areas are likely to emerge
- Need to explore advanced computer architectures and systems software



### What's New for SciDAC-2?

- Learn from SciDAC's successes to date
- Additional areas of emphasis
  - University-based SciDAC institutes
  - Experimental science
- New Partners and/or Application Domains
- Single Program Notice
- Applications submitted by universities through grants.gov
- Laboratory proposals submitted through ePMA (formerly ePME)



# Scientific Discovery through Advanced Computing...

**Advanced Scientific Computing Research Program** 

### SciDAC-2 initiated in 4<sup>th</sup> Qtr FY 2006, will create:

- Comprehensive, scientific computing software infrastructure-integrating applied mathematics, computer science and computational science for scientific discovery at the petascale
- New generation of data management and knowledge discovery for large scientific data sets

#### Partners:

- Office of Science (\$66M)
- National Nuclear Security Administration (\$4M)
- National Scientific Foundation (TBD)



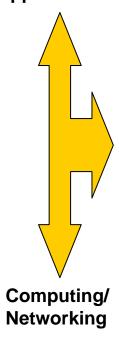
## SciDAC-2 Timeline

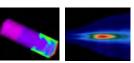
Date	Event	Comments
December 23, 2005	Call for Proposals	Notice to Universities for Grants Announcement to Laboratories for Proposals
January 23, 2006	Letters of Intent Due	Over 350 submitted; 270 encouraged
March 6, 2006	Proposals Due	110-lab lead; 120-university-lead; grants.gov, ePMA and PDF
April 10-21, 2006	Panel Reviews	15 panels, some mail reviews; cross-cut panel
July 3, 2006	Grant Actions to Chicago	Needed to ensure FY2006 start
TBD	Awards Announced	

# SciDAC-2 -- Leading the Way to Petascale --

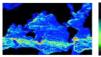
## Scientific Discovery

### Applications





















- Accelerator science and simulation
- Climate modeling and simulation
- Fusion science
- Petabyte high-energy/nuclear physics
- Nuclear physics
- Radiation transport

- Astrophysics
- Computational Biology
- High-energy physics
- Materials science and chemistry
- QCD
- Turbulence
- Groundwater reactive transport modeling and simulation



- Centers for Enabling Technology

- Scientific Applications Partnerships

- Institutes (University-lead)

**Leadership Computing- ANL** 

**Leadership Computing-**

**ORNL** 

100 TF

250 TF

**Production Computing-**

**NERSC** 

100-150 TF

**ESnet** 

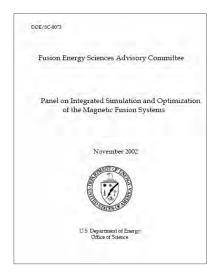
On path toward Dual rings 40Gbps/ 10 Gbps fault tolerant

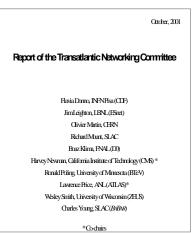


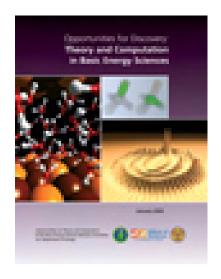




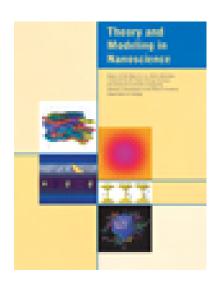
### Requirements for High Performance Computing and Networks Continue to Increase

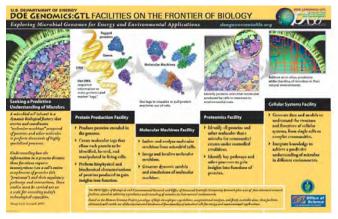








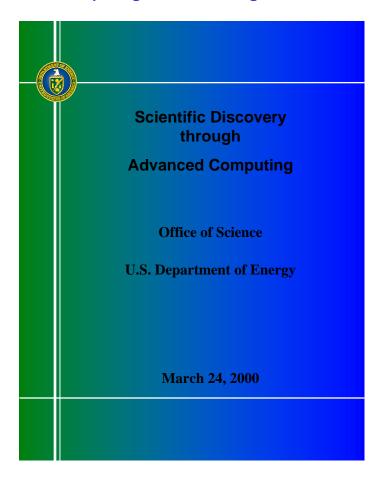






### SciDAC Plan

**Advanced Scientific Computing Research Program** 



On March 30, 2000 the Office of Science submitted a plan for scientific computing to the Energy & Water Development Subcommittees of the Appropriations Committees of the U.S. Congress.

The plan, titled "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 its research programs in basic energy sciences, biological and environmental research, fusion energy sciences, and high energy and nuclear physics.

URL: http://www.scidac.org/SciDAC.pdf



# SciDAC Goals -- as articulated in FY 2001 --

- An integrated program to:
- Create a new generation of Scientific Simulation Codes that take full advantage of the extraordinary computing capabilities of terascale computers.
  - Create the Mathematical and Computing Systems
     Software to enable the Scientific Simulation Codes to
     effectively and efficiently use terascale computers.
  - Create a Collaboratory Software Environment to enable geographically separated scientists to effectively work together as a team and to facilitate remote access to both facilities and data.



### SciDAC Effectiveness

**Advanced Scientific Computing Research Program** 

OMB Measure: Improve Computational Science Capabilities.
 Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the Scientific Discovery through Advanced Computing.

#### Feedback:

- Steve Jardin (PPPL): "... [SciDAC] is a significant factor in our productivity, comparable to that obtained by going to the next-generation computer."
- Tony Mezzacappa (ORNL): "The SciDAC Program is making possible a whole new class of supernova simulations. I could never go back to singleinvestigator research."
- Rob Ryne (LBNL): SciDAC algorithmic advancements and visualization in accelerator design enable us to "... optimize designs to reduce costs and risks and help ensure project success."