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

DOE's Vision for Computational Science

by
Dr. Raymond Orbach
Director, Office of Science

President's Information Technology Advisory Committee
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Board Room
National Science Foundation

presented by
Dr. Michael Strayer
Director, SciDAC

High-end Computation at the Forefronts of Science

Essential tool in all areas of the Office of Science:

- Accelerator Design
- Astrophysics
- Biology
- Chemistry
- Climate Modeling
- Combustion
- Fusion Energy
- Nanoscience
- Nuclear Physics
- Quantum Chromodynamics

Computational Science as a Methodology

Computational Science is an indispensable third pillar of scientific inquiry complementing theory, observation, and experiment

As science's newest tool, it holds great promise for resolving outstanding difficult questions and opening up new territories for exploration

We are pursuing computational science as a unifying theme across the entire Office, through the SciDAC program

U.S. Department of Energy

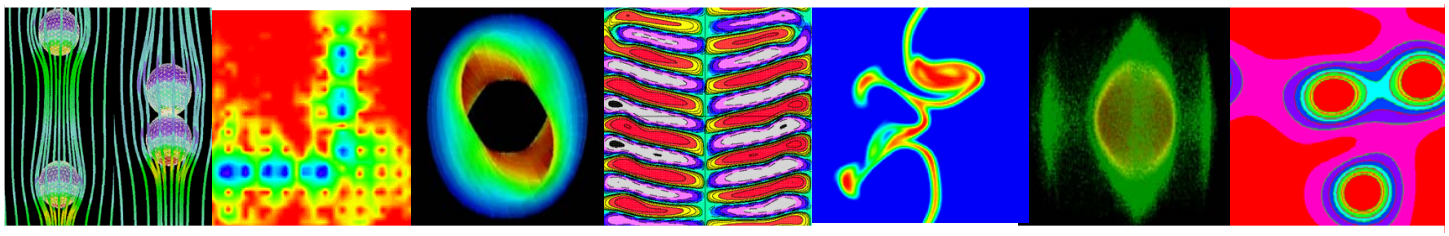
Office of Science

SciDAC

SciDAC
Scientific Discovery through Advanced Computing

Scientific Discovery through Advanced Computing

www.science.doe.gov/scidac



SciDAC

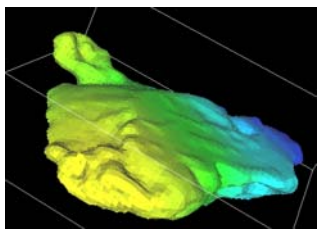
SciDAC
Scientific Discovery through Advanced Computing

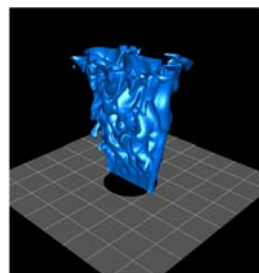
An integrated program

Take advantage of capabilities of terascale computers by creating a new generation of applications codes that take science into new territories

Create the mathematical algorithms and computing systems software to enable scientific simulation codes to effectively and efficiently use terascale computers

Enable geographically distributed scientists to work effectively together as *teams* and to facilitate remote access to unique high-end resources





Benefits of SciDAC

Benefits of *"team-based science"* are both technical and sociological

Synergistic benefits derived from interdisciplinary interactions

(e.g. Community Climate System Model)

SciDAC multi-institutional teams with enhanced collaborations have increased performance

High-End Computing Resources

SciDAC computing and networking resources are provided principally by the *Office of Advanced Scientific Computing Research*

This includes *both* *capacity* and *capability* resources

Capacity Resources

Capacity resources include:

Machine	Technology	Use	Processors	CPU[(1)] Hours
Seaborg	IBM Power-3	General	6176	48.7 million
Eagle	IBM Power-3	Climate	704	5.5 million
Cheetah	IBM Power-4	General	768	6.1 million
MPP2	HP Intel Itanium	Environment	1900	0.75 million

High-End Computing Resources

Capability resources being established through the Leadership-Class Computing Initiative

- Cray: X1, Red Storm, Black Widow
- IBM: Blue Gene
- SGI: Altix

Capability goal is one sustained petaflop by the end of this decade

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Capability Resources

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Capability resources being established through the Leadership-Class Computing Initiative

Develop and evaluate next-generation architectures with industry

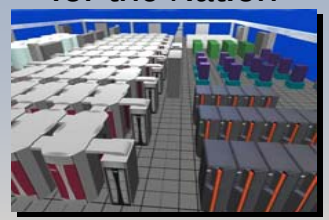
IBM

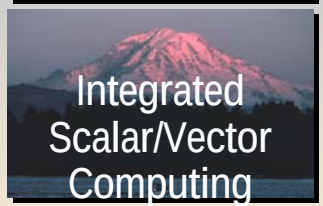
SRC

CRAY

sgi

Provide leadership-class computing resources for the Nation





Create math and CS methods to enable use of resources

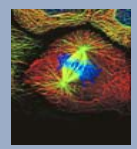
SciDAC ISICs

Scientific Applications Partnerships

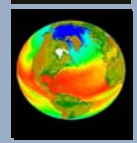
Modeling and simulation expertise

Transform scientific discovery through advanced computing

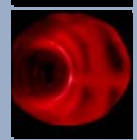
Computational End Stations



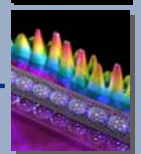
Biology



Climate



Fusion



Materials

Industry/ other agencies

Capability Resources

"Capability goal is one sustained petaflop by the end of this decade"

Collaboration & Outreach

Office of Science is working with the interagency community and the National Coordination Office to ensure that high-end computing resources are needs-driven and available to all

Partnerships with universities are the rule within the Office of Science – and especially so in SciDAC

Vigorous outreach and pre-competitive technology research projects with applications industries are planned

INCITE

10% of Seaborg made available to the scientific community for high impact science.

No requirement for direct relationship to Office of Science programs.

Encourage the development of a new sociology for high-end computation.

- 4.5M CPU hours available
- 53 proposals received
- 130.5M CPU hours requested
- 65% from U.S. academic institutions
- 12 different scientific disciplines
- 62% for research not funded by DOE

INCITE

SciDAC Scientific Discovery through Advanced Computing

Three Awards

"Thermonuclear Supernovae: Stellar Explosions in Three Dimensions," Tomasz Plewa, Center for Astrophysical Thermonuclear Flashes, University of Chicago (2.7 M).

"Fluid Turbulence and Mixing at High Reynolds Number," Professor P. K. Yeung, Georgia Institute of Technology (1.2 M) [current support from the NSF].

"Quantum Monte Carlo Study of Photoprotection via Carotenoids in Photosynthetic Centers," William A. Lester, Jr., Lawrence Berkeley National Laboratory and the University of California Berkeley (1 M).

The Path Foreword

What are scientific needs and priorities for high performance computing?

How well do these requirements match existing and future system architectures ?

What are the opportunities for expanded HPC applications?

What are the drivers or constraints to expanded HPC usage?

Insight

The purpose of computing is insight, not numbers.

Richard W. Hamming
Numerical Methods for Scientists and Engineers, 1973