

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

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Scientific Discovery through Advanced Computing (<http://www.scidac.gov/>)

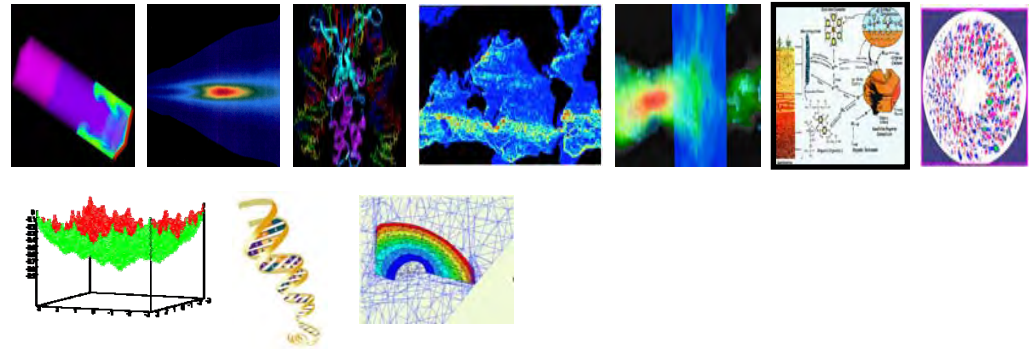
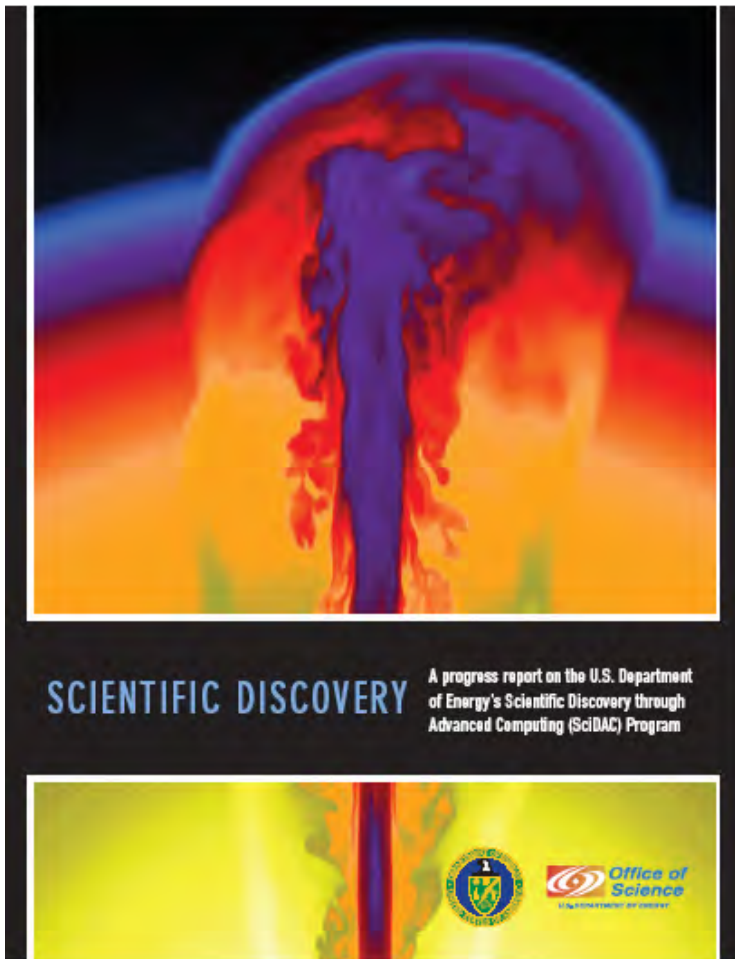
## Scientific Discovery through Advanced Computing -- Update --

**Walter M. Polansky**  
Advanced Scientific  
Computing Research Program



# SciDAC Successes 2001 - 2006

Scientific Discovery through Advanced Computing



Publications	
2001	94
2002	186
2003	277
2004	247
2005-06	377



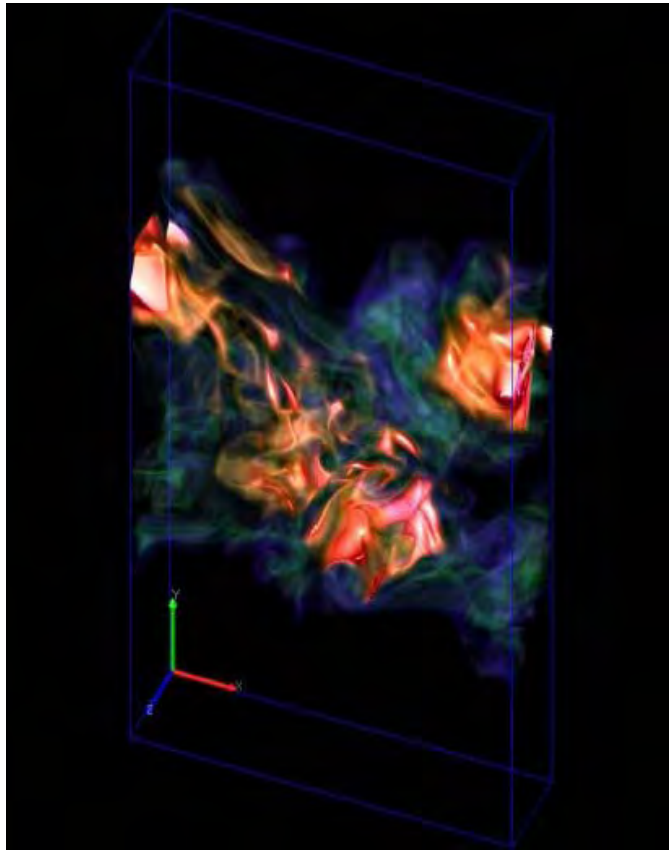
<http://www.scidac.gov/>



# Celebrating Success

## (Recent SciDAC Accomplishments)

### Scientific Discovery through Advanced Computing



*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 Review and Scientific Discovery document numerous SciDAC accomplishments



# SciDAC Goals

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Scientific Discovery through Advanced Computing

- **Create comprehensive, scientific computing software infrastructure to enable scientific discovery in the physical, biological, and environmental sciences at the petascale**
- **Develop new generation of data management and knowledge discovery tools for large data sets (obtained from scientific user and simulations)**

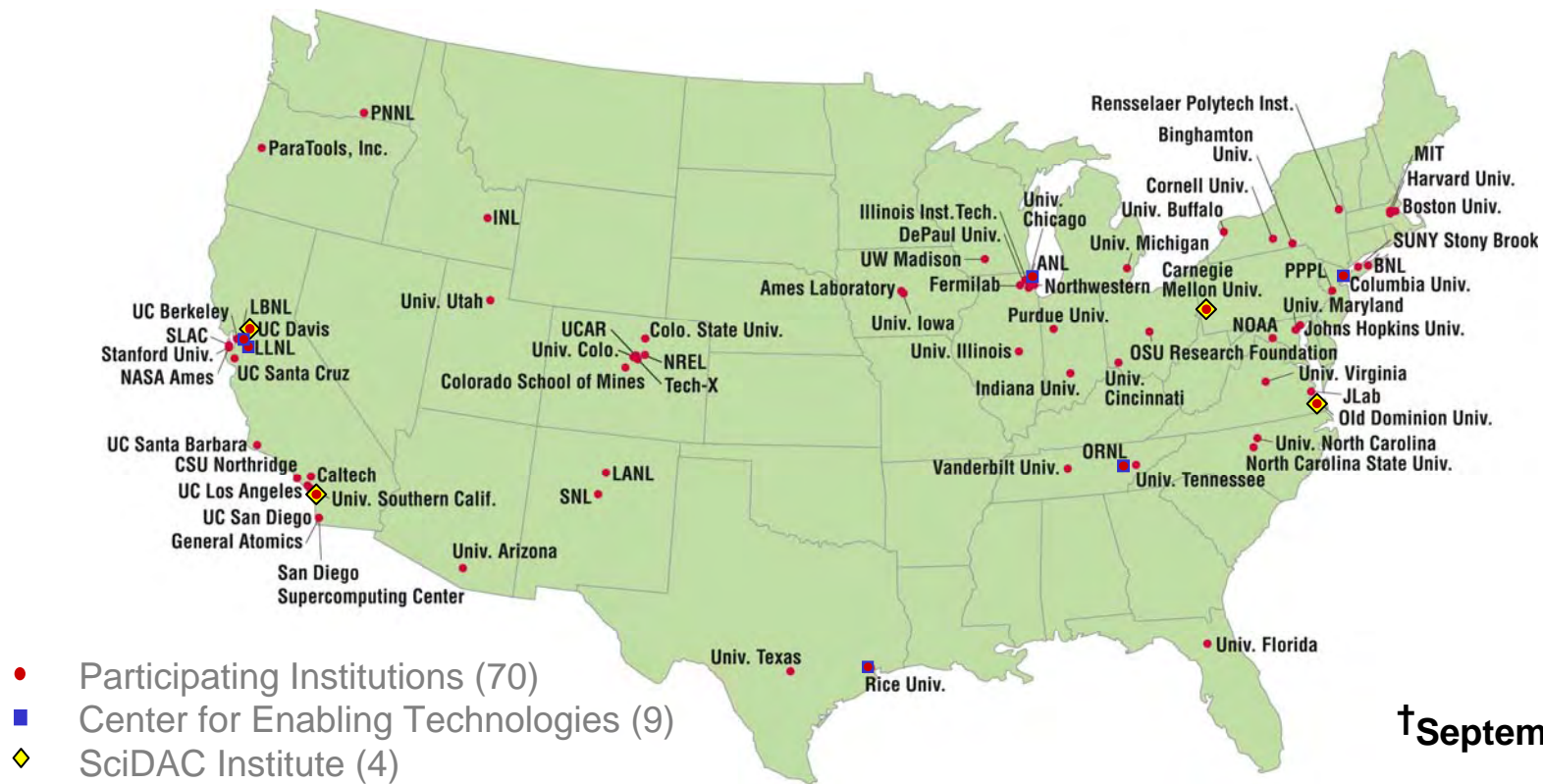


# SciDAC-2 Awards

(<http://www.energy.gov/news/4135.htm>)

Scientific Discovery through Advanced Computing

Today<sup>†</sup>, the Department of Energy's Office of Science is announcing approximately \$60 million in new SciDAC-2 awards annually for 30 computational science projects over the next three to five years





# SciDAC

Scientific Discovery through Advanced Computing

Computational Collaborations to Drive Scientific Discovery

## Statistics

**31- SciDAC projects**

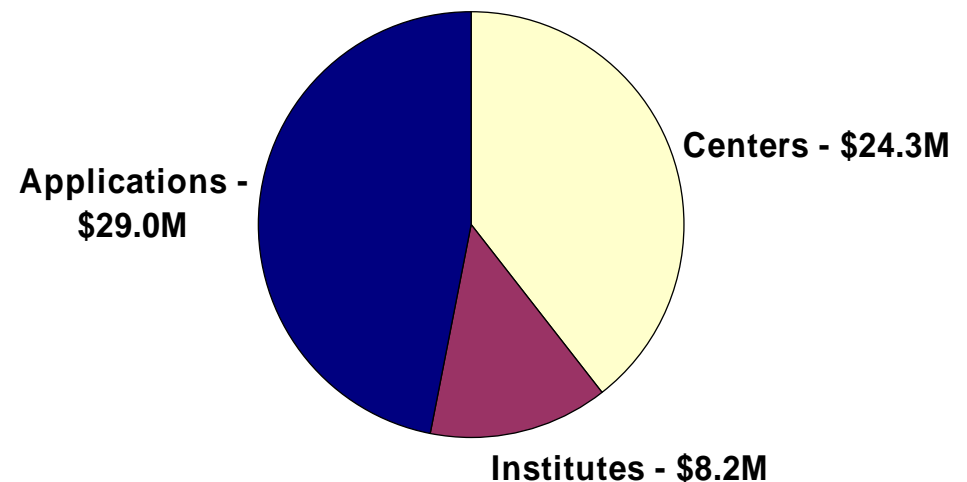
**9- Centers**

**4- Institutes**

**18- Efforts in 11 application areas**

*Astrophysics, Climate, Biology,  
Fusion, Petabytes, Materials &  
Chemistry, Nuclear physics, High  
Energy physics, QCD, Turbulence,  
Groundwater*

**New performers ? About 60% of the  
funds !**



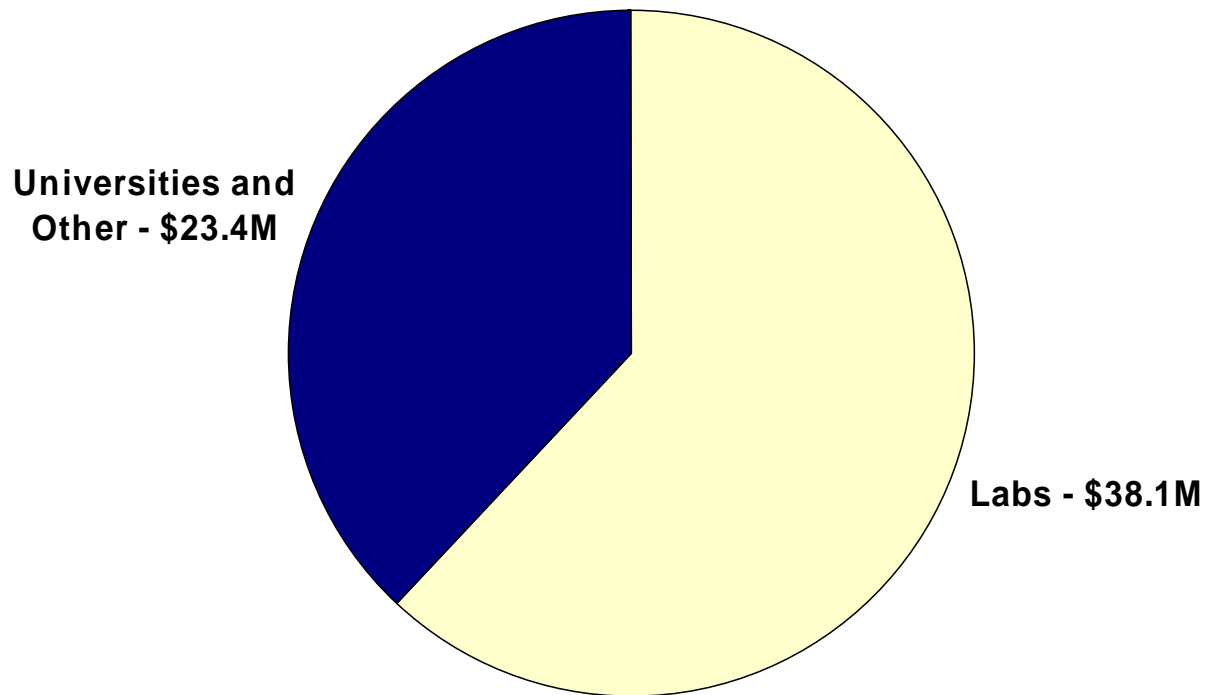
**Total- \$61.5 M**



# SciDAC Participants

Scientific Discovery through Advanced Computing

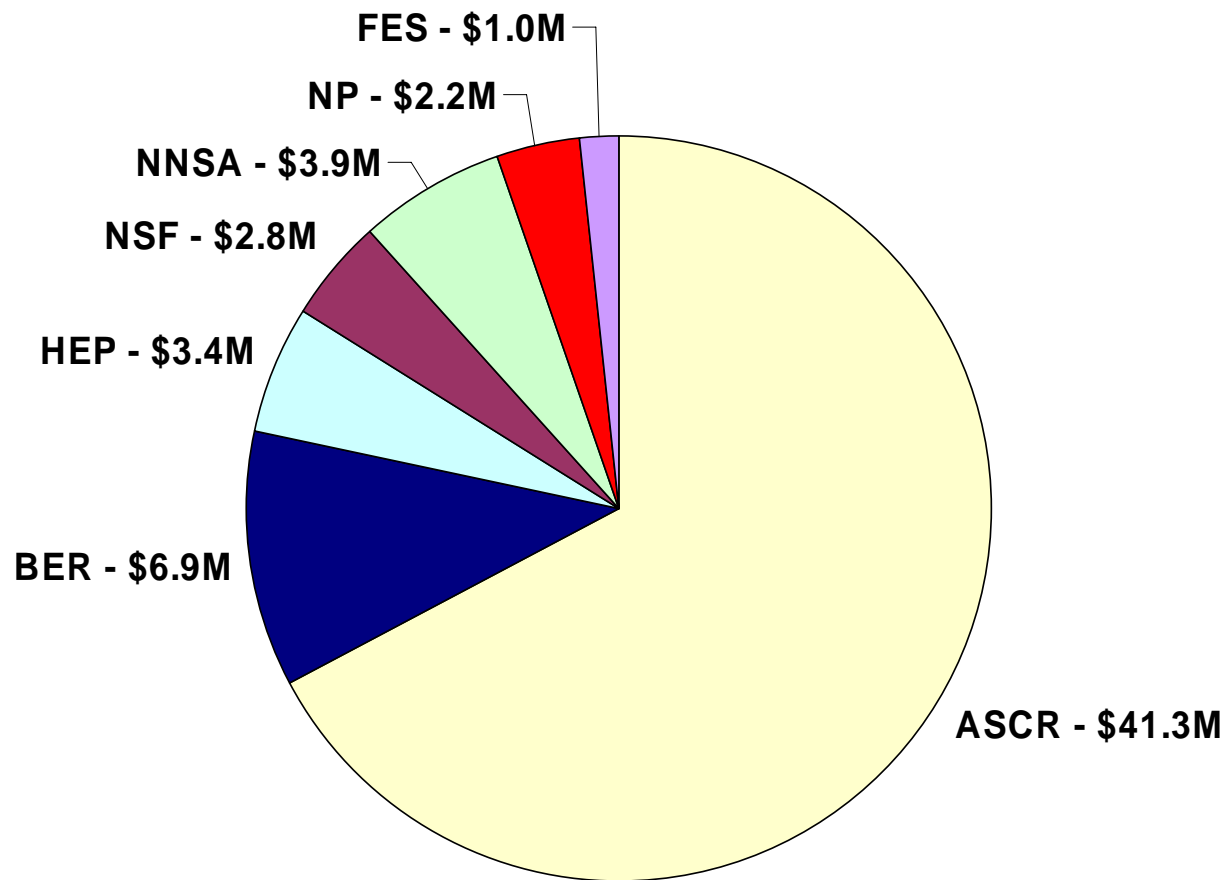
**17 Laboratories (15-DOE; 1- NASA; 1- NOAA)**  
**55 Universities**  
**3 Companies**





# Funding Sources

Scientific Discovery through Advanced Computing





*U.S. Department of Energy*



*Office of Science*

Scientific Discovery through Advanced Computing

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# Centers and Institutes



# Institutes and Centers -- Attributes --

Scientific Discovery through Advanced Computing

- **Institutes- University-led centers of excellence**
  - Focus on major software issues
  - Employ range of collaborative research interactions.
  - Reach out to engage a broader community of scientists in scientific discovery through advanced computation and collaboration.
  - Conduct training/outreach in high performance computing topics.
- **Centers for Enabling Technology- work directly with applications:**
  - Develop to enable scientific simulation codes to take full advantage of tera- to peta-scale.
  - Ensure critical computer science and applied mathematics issues are addressed in a timely and comprehensive fashion.
  - Address issues associated with research software lifecycle.



# Centers & Institutes

-- Applied Mathematics --

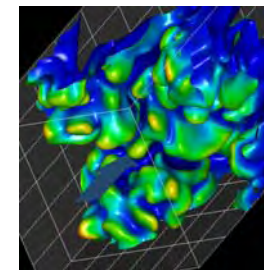
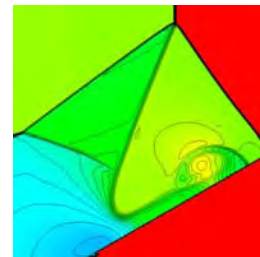
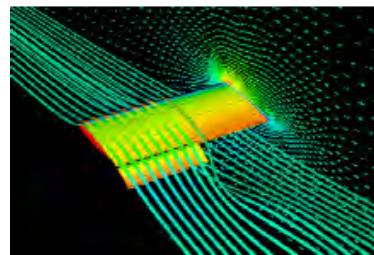
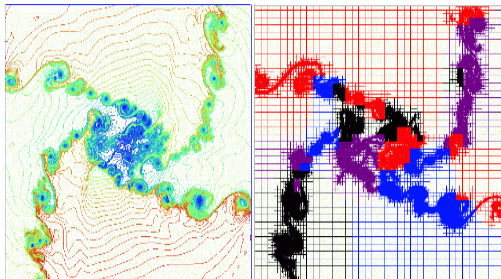
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## Centers:

- **APDEC** - Finite difference/finite volume methods, adaptive mesh refinement, multiresolution. PI: Phillip Colella. (3 labs.)
- **ITAPS** - Mesh, geometry, field manipulation tools. PI: Lori Diachin. (5 labs, 3 universities.)
- **TOPS** - Mathematical software infrastructure for scalable PDE solvers. PI: David Keyes. (4 labs, 9 universities.)

## Institutes:

- **CSCAPES**- Load balancing, parallelization toolkits, sparse matrix software, combinatorics, hypergraphs. PI: Alex Pothen. 2 universities, 2 labs.



# Centers and Institutes -- Computer Science --

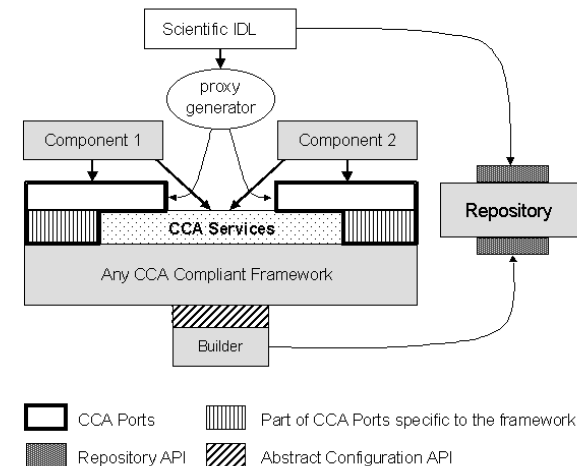
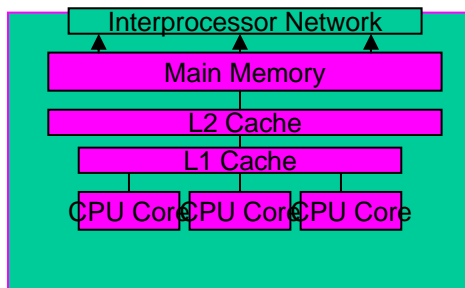
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## Centers:

- **CSADS** - Open source high performance multicore compiler infrastructure. PI: Ken Kennedy. 1 lab, 4 universities.
- **TASCS** - Advanced component software, common component architecture. PI: David Bernholdt. 6 labs, 5 universities

## Institutes:

- **PDSI** - Petascale data storage and high performance file systems. PI: Garth Gibson. 5 labs, 3 universities.
- **PERI** - Automatic performance measurement and optimization. PI: Robert Lucas. 4 labs, 6 universities.





# Centers and Institutes Distributed Computing/Visualization

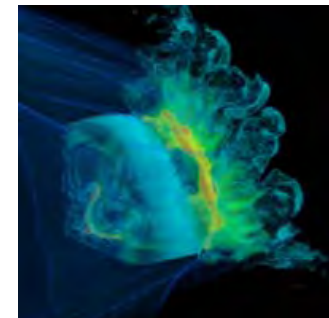
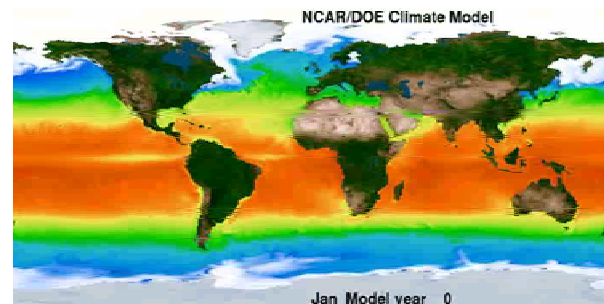
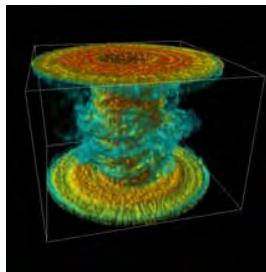
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## Centers:

- **CEDPS** - High performance services and tools for distributed scientific data management. PI: Ian Foster. (3 labs, 2 universities.)
- **ESG** - Earth systems grid support for petascale climate data. PI: Dean Williams. (7 labs, 1 university.)
- **SDM** - Scientific data management framework for petascale computation. PI: Arie Shoshoni. (5 labs, 5 universities.)
- **VACET** - Scientific data visualization and analytics. PI: Wes Bethel. 3 labs, 2 universities.

## Institutes:

- **UVIS** - High performance parallel visualization strategies. PI: Kwan-Liu Ma. (2 labs, 4 universities.)





# SciDAC Challenges

-- Operational and Management --

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Scientific Discovery through Advanced Computing

- **Provide a fertile environment for scientific discovery through modeling and simulation**
- **Make SciDAC resources available to the broad research community.**
- **Communicate SciDAC model**
- **Optimize relationships between and/or among**
  - **CETs and applications**
  - **CETs with each other**
  - **Institutes, CETs and applications**



# SciDAC Outreach Center David Skinner, PI

Scientific Discovery through Advanced Computing

- **Innovative web and software services**
  - Tools which make SciDAC researchers more effective at delivering their technologies (web hosting and authenticated wiki-like portals)
  - Services to promote an easy interface between SciDAC and ‘the outside computational world’ (web, email, and phone central point of contact for SciDAC inquiries)



- **Workshops, training sessions**
  - Getting the right people together to forge collaborations

**Build Collaborations to Drive Scientific Discovery**

([outreach.scidac.gov](http://outreach.scidac.gov); [help@outreach.SciDAC.gov](mailto:help@outreach.SciDAC.gov))



# SciDAC Outreach -- Status --

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## Scientific Discovery through Advanced Computing

- **Managed SciDAC PI Workshop (February 5-6, 2007, Atlanta)**
  - Documented 54 existing collaborative connections between CETs and SAPs
  - Identified 65 more potential specific resource/need matches to develop
  - Collected 12 points of contact for inquiries on specific topics
- **Fielded questions by phone or email**
  - 14 substantive interactions so far
  - “Can SciDAC support my application development?” – Application Scientist
  - “How is my institution involved with SciDAC” – Campus communications staff
  - “Do you know if there will be a BOF session on X at conference Y?” – SciDAC Researcher
  - “Please announce our workshop.” – SciDAC PI
  - “Who might be interested in our switch technology” – Vendor
  - “We have a storage solution that may be of interest to Scientists.” – Vendor





# SciDAC Solicitations FY2007

Scientific Discovery through Advanced Computing

- **Climate Change Prediction Program Notice Closed- January 25, 2007; (BER)**  
(<http://www.science.doe.gov/grants/FAPN07-06.html>)
  - “...contribute to a measurably improved ability to computing infrastructure to address challenging problems in climatic change science.”
- **Accelerator Science and Simulation; Closed- January 17, 2007; (HEP, NP, BES and ASCR)**  
(<http://www.science.doe.gov/grants/FAPN07-09.html>;  
[http://www.science.doe.gov/grants/LAB07\\_09.html](http://www.science.doe.gov/grants/LAB07_09.html))
  - “...computational approach for interacting with the SciDAC Institutes and Centers for Enabling Technologies.”

# Conference

SciDAC 2007 Conference - Microsoft Internet Explorer provided by The Office of Science

File Edit View Favorites Tools Help

Address <http://www.scidac.gov/Conference2007/> Go

## SciDAC 2007

Scientific Discovery through Advanced Computing  
June 24 - 28 Boston



Registration will begin  
February 2007



### SciDAC 2007

The Scientific Discovery through Advanced Computing Program (SciDAC) operated by the Department of Energy Office of Science has begun its second round of projects, after a wealth of successful projects. This unique program has brought together computational scientists from across the world.

- Home
- Organizing Committee
  - OC only
- Registration
- Lodging
- Agenda