

U.S. Department of Energy



Office of Science

Advanced Scientific Computing Research Program

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

Scientific Discovery through Advanced Computing

-- Update --

Walt Polansky

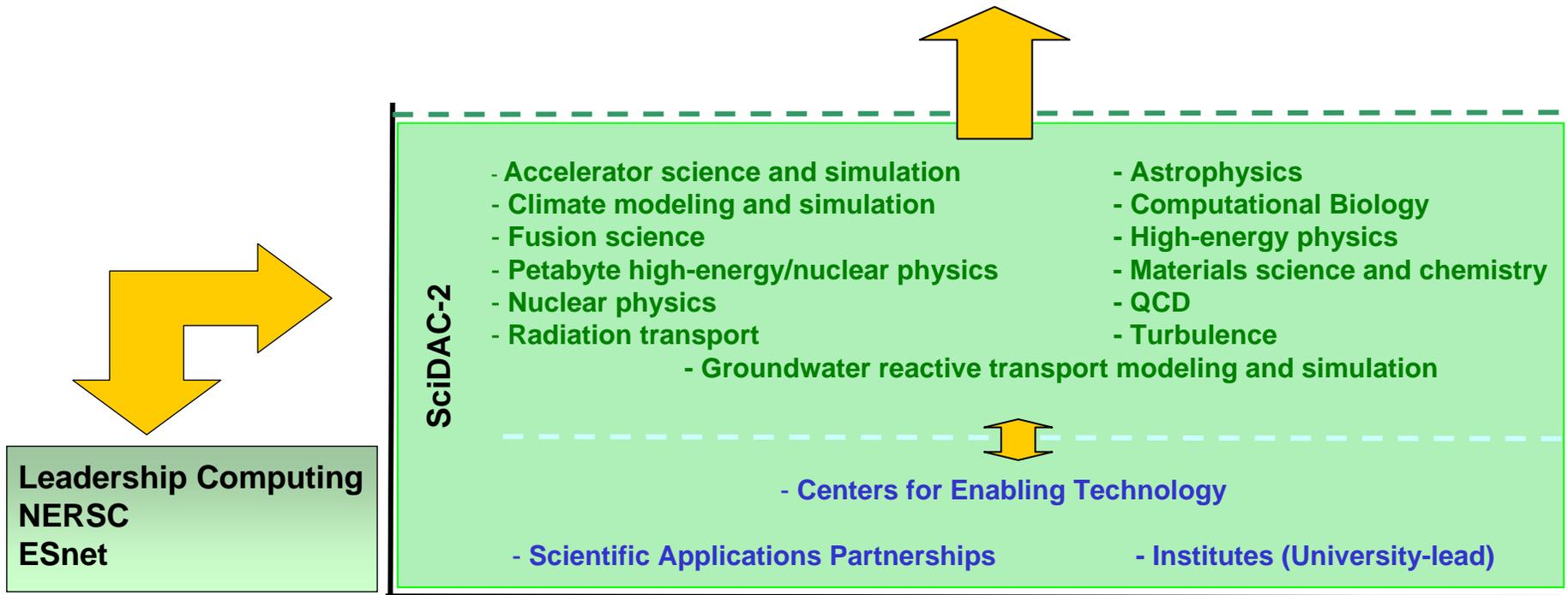
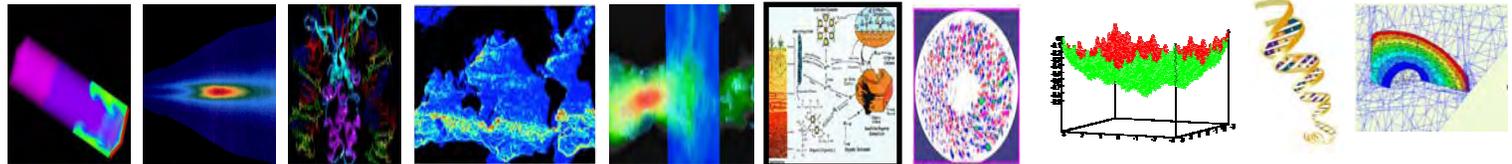
Walt.Polansky@Science.doe.gov

301-903-5935



Scientific Discovery -- Through Modeling and Simulation --

Advanced Scientific Computing Research Program





SciDAC-2 Institutes...

- ... **University-led centers of excellence that focus on major software issues through a range of collaborative research interactions.**
 - Develop, test, maintain, and support optimal algorithms, programming environments, systems software and tools, and applications software.
 - Focus on a single general method or technique.
 - Focal point for bringing together a critical mass of experts from multiple disciplines to focus on key problems in a particular area of enabling technologies.
 - Forge relationships between experts in software development, scientific application domains, high performance computing, and industrial partners.
 - **Reach out to engage a broader community of scientists in the activities of scientific discovery through advanced computation and collaboration.**
 - **Incorporate training and outreach in high performance computing topics, including for graduate students and postdocs.**

Funding source- ASCR program



Centers for Enabling Technologies... (CETs)

Advanced Scientific Computing Research Program

- ... **provide the essential computing and communications infrastructure to support SciDAC applications; multi-discipline approach with activities in:**
 - Algorithms, methods, and libraries.
 - Program development environments and tools -- terascale and petascale program development and tools provide maximum ease-of-use to scientific end users.
 - Systems software that provides system stability and functionality needed by users for tera- to peta- scale simulations.
 - Visualization and data management systems.
- **CETs work directly with applications on:**
 - Development and application of computing systems software that allows scientific simulation codes to take full advantage of the extraordinary capabilities of terascale and petascale computers.
 - Ensuring that the most critical computer science and applied mathematics issues are addressed in a timely and comprehensive fashion.
 - Addressing all aspects of the successful research software lifecycle including transition of a research code into a robust production code and long term software evolution and maintenance and end user support.

Funding Source- ASCR Program



Science Applications

- **Goals**
 - **Achieve breakthrough scientific advances through computer simulation that**
 - **are impossible using theoretical or experimental studies alone**
or
 - **improve experimental science.**
- **Funding Source(s)**
 - **Office of Science programs (ex. ASCR), NNSA or NSF, either individually, jointly and ASCR if:**
 - **Application teams include applied mathematicians or computer scientists.**



SciDAC-2 -- Status Report --

- **Final preparations underway to support the announcement of the SciDAC-2 portfolio**
 - Centers for Enabling Technologies
 - Institutes
 - Science Applications
- **About 250 separate funding actions, currently in negotiation, will be made by DOE on SciDAC-2.**
- **In addition to the Office of Science, NNSA and NSF will be funding SciDAC-2 research efforts.**
- **Many SciDAC-2 projects could start work as soon as mid-September, 2006**



SciDAC-2 Proposal Review Process

- **Mail peer reviews**
 - Radiation Transport, Nuclear Physics, and Lattice Quantum Chromodynamics
- **Peer review panels**
 - Material Science, Biology, Climate, Turbulence, Groundwater, Fusion, Astrophysics, Physics with Petabytes, and Accelerator Physics.
- **Crosscut Panel- portfolio quality, breadth and compatibility with SciDAC-2 vision**

U.S. Department of Energy



Office of Science

Advanced Scientific Computing Research Program

SciDAC-2 Review Panel Guidance- Example

Scientific Discovery through Advanced Computing

Notice 06-04 and Lab Announcement 06-04

Panel B-7
Computer Science
SciDAC Institutes
Tuesday April 18, 2006



SciDAC-2 Review Panel Guidance- Example

SciDAC-2 Scope

- **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)**

Notice- <http://www.sc.doe.gov/grants/FAPN06-04.html>
Announcement- http://www.sc.doe.gov/grants/LAB06_04.html



SciDAC-2 Review Panel Guidance- Example

Advanced Scientific Computing Research Program

Review Criteria

-- in the context of SciDAC-2 --

- Scientific/Technical Merit
- Appropriateness of Proposed Method or Approach
- Competency of personnel
- Adequacy of proposed resources
- Reasonableness and appropriateness of budget

<u>Score</u>	<u>Description</u>
9-10	Excellent- 'cream of the cream'
7-8	Very good 'Fundable' to 'Top echelon'
5-6	Good 'on the margin'
0-4	Poor to Fair 'don't consider'

Laboratory led submissions reviewed separately from University led submissions



SciDAC-2 Cross-cut Panel

Charter

- Comment on overall quality of the SciDAC-2 peer review process;
- Identify/comment on proposals that could be candidates for funding, using peer reviews, professional experience and program manager comments, when provided.
- Offer a perspective on the quality, the breadth and the balance represented by the Top Rated proposals within each major SciDAC category (Science Applications, CETs and Institutes)
- Comment on the overall quality and synergism of a SciDAC portfolio comprised of all Top Rated proposals.

Panelists' reports (submitted individually) were forwarded to DOE SciDAC program managers.



SciDAC Management -- Near Term Actions --

Advanced Scientific Computing Research Program

- **Establish a capability to make SciDAC resources available to the entire research community involved in computational science**
- **Institutes**
 - Procedures for out-reach to non-SciDAC research areas
 - Training
- **Centers for Enabling Technologies**
 - Interfaces with Applications and each other; management plans