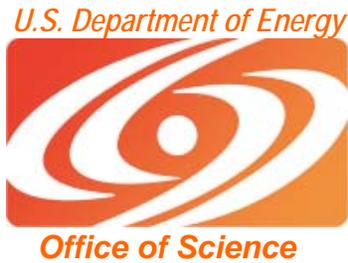# Scientific Discovery through Advanced Computing

-- Update & Review Plans --

ASCAC Meeting
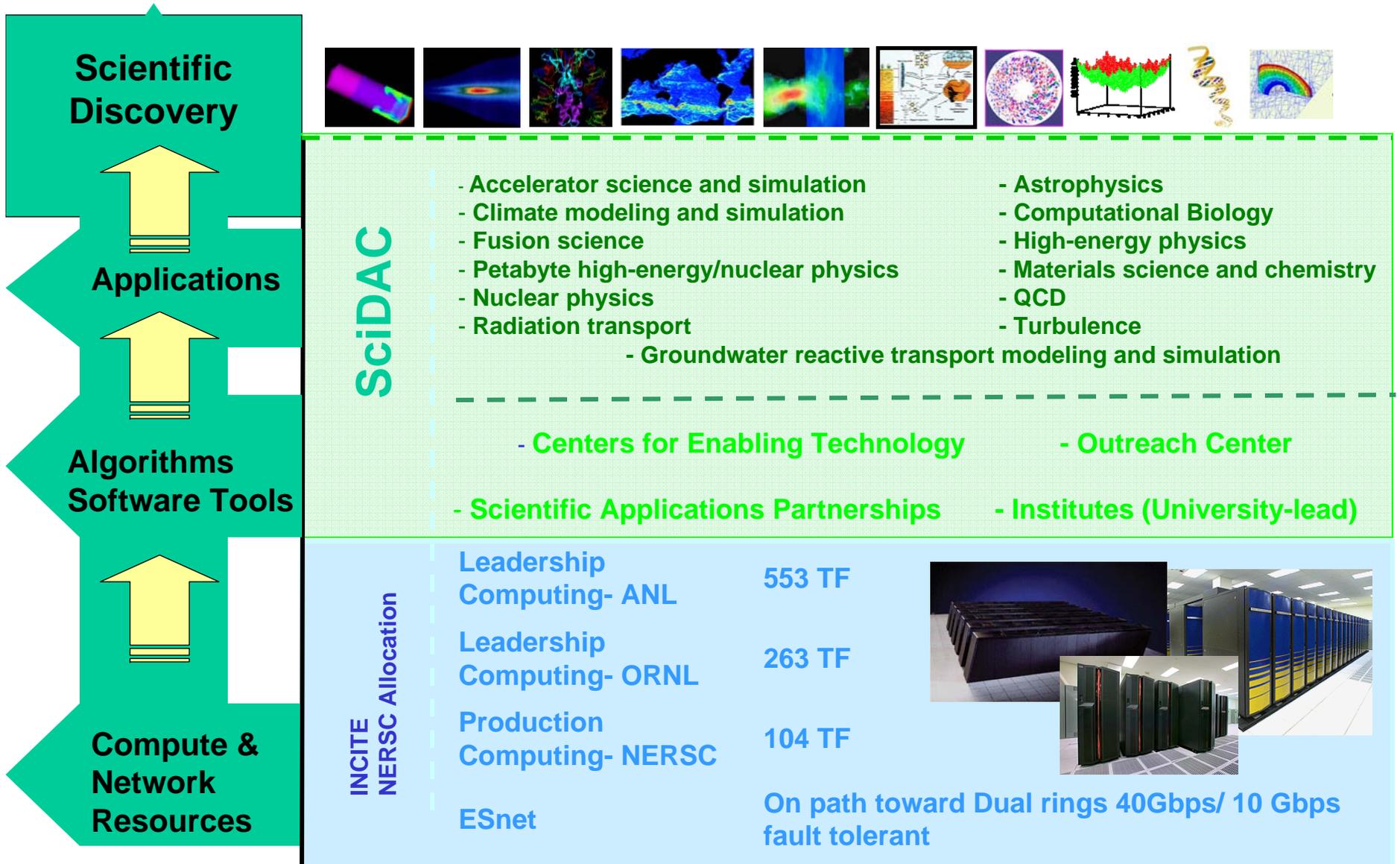**October 28-29, 2008**
Gaithersburg, MD

Walter M. Polansky
Acting Director
Computational Science
Research and Partnerships Division

SciDAC-2 Goals

- **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)**

Scientific Discovery through Advanced Computing

Scientific Discovery

Applications

Algorithms Software Tools

Compute & Network Resources

SciDAC

- 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**   - **Outreach Center**

- **Scientific Applications Partnerships**   - **Institutes (University-lead)**

INCITE NERSC Allocation

Leadership Computing- ANL   553 TF

Leadership Computing- ORNL   263 TF

Production Computing- NERSC   104 TF

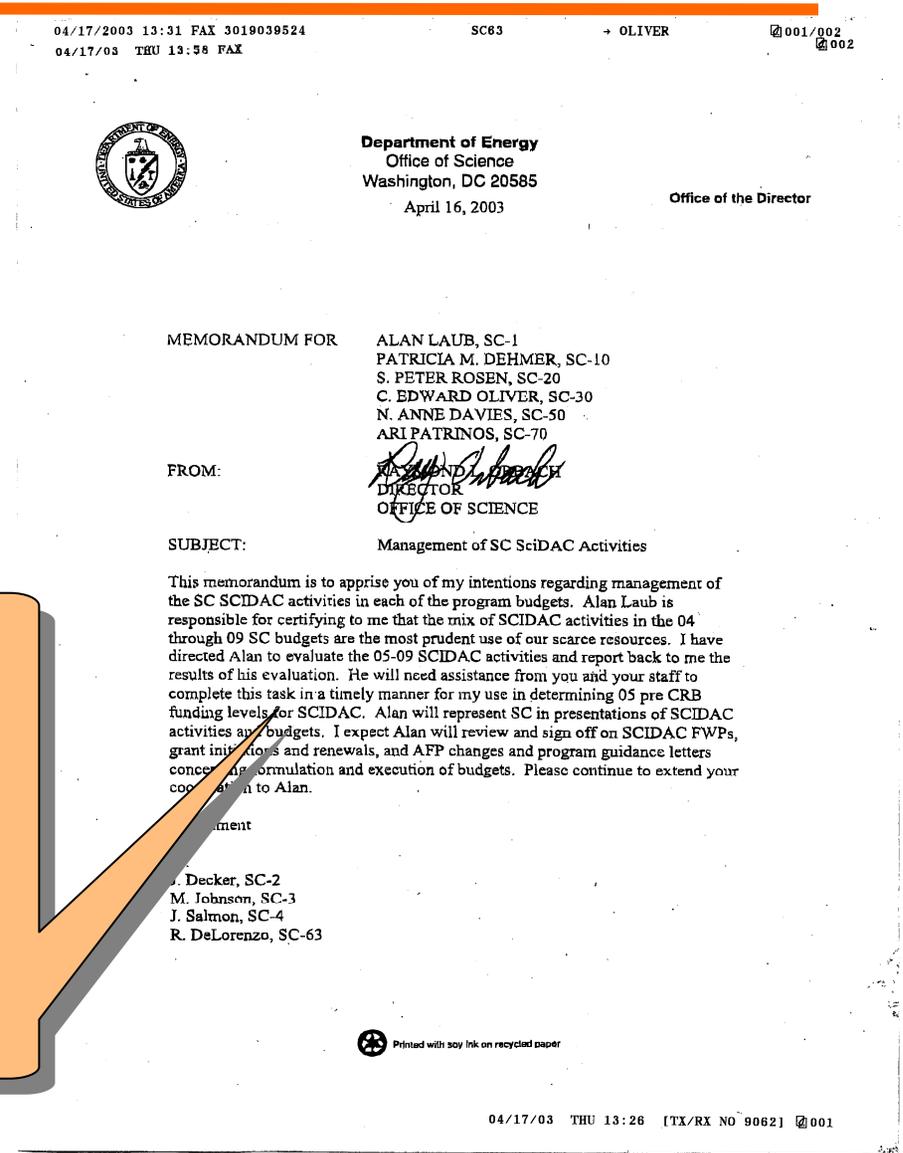ESnet   On path toward Dual rings 40Gbps/ 10 Gbps fault tolerant

SciDAC Management Policy
-- Established April 16, 2003 --

- **Memorandum states Dr. Orbach's intentions regarding management of SC SciDAC activities in each of the program budgets.**
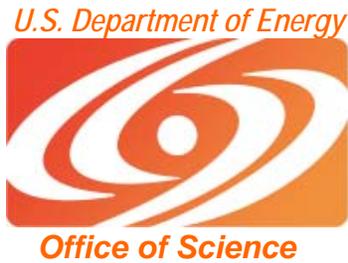
- **Michael R. Strayer is the SciDAC Director**

> **"Expect SciDAC Director to review and sign-off on SciDAC FWPs, grant initiations and renewals,and AFP changes and program guidance letters concerning formulation and execution of budgets."**

04/17/2003 13:31 FAX 3019039524   SC63   → OLIVER   001/002
04/17/03 THU 13:58 FAX   002

Department of Energy
Office of Science
Washington, DC 20585   **Office of the Director**

April 16, 2003

MEMORANDUM FOR   ALAN LAUB, SC-1
                   PATRICIA M. DEHMER, SC-10
                   S. PETER ROSEN, SC-20
                   C. EDWARD OLIVER, SC-30
                   N. ANNE DAVIES, SC-50
                   ARI PATRINOS, SC-70

FROM: RAYMOND L. ORBACH
                   DIRECTOR
                   OFFICE OF SCIENCE

SUBJECT: Management of SC SciDAC Activities

This memorandum is to apprise you of my intentions regarding management of the SC SCIDAC activities in each of the program budgets. Alan Laub is responsible for certifying to me that the mix of SCIDAC activities in the 04 through 09 SC budgets are the most prudent use of our scarce resources. I have directed Alan to evaluate the 05-09 SCIDAC activities and report back to me the results of his evaluation. He will need assistance from you and your staff to complete this task in a timely manner for my use in determining 05 pre CRB funding levels for SCIDAC. Alan will represent SC in presentations of SCIDAC activities and budgets. I expect Alan will review and sign off on SCIDAC FWPs, grant initiations and renewals, and AFP changes and program guidance letters concerning formulation and execution of budgets. Please continue to extend your cooperation to Alan.

cc:
J. Decker, SC-2
M. Johnson, SC-3
J. Salmon, SC-4
R. DeLorenzo, SC-63

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Review of SciDAC Portfolio

- ## Timeline
  - **Science Applications: Jan – April, 2009**
  - **Centers and Institutes: April - May, 2009**

- ## Process
  - **Peer Review (with Panels)**
  - **Reviewer Selection:**
    - Science Applications: Funding office(s), in partnership with ASCR
    - CETs, Institutes and Outreach Center: ASCR, in consultation with other SC offices, NNSA and/or NSF.

SciDAC Coordination Group

Comprised of Program managers from ASCR, BER, BES, FES, HEP, NP, and NNSA

(ASCR SciDAC Team- Lali Chatterjee, Christine Chalk, Bill Spotz, Osni Marques, Susan Turnbull, Walt Polansky)

- **Formulated Notice and Announcement**
- **Managed peer reviews**
- **Recommended projects for funding**
- **Prepared award packages**
- **Managed awarded projects**

- **Developing procedures for organizing, scheduling and conducting peer reviews of the SciDAC portfolio.**

Review Schedule
-- Tentative --

Project Title	PI, Inst	Timelines	Partners	Review schedule	Participants
Framework Application for Core-Edge Transport Simulations (FACETS)	J Cary, Tech X	Project '11, SAP 09	FES (Lead), ASCR	May, 2009 (DC)	4 labs, 4 universities, 3 industry
Computational Astrophysics Consortium: Supernovae,………	S Woosley, UC Santa Cruz	Project '11, SAP 09	HEP (Lead), NP, NNSA, ASCR	Jan 21-22, 2009 (CA)	3 labs, 5 universities
A…... Earth System Model for Climate Change Science	J Drake, ORNL	Project '11, SAP 09	BER (Lead), ASCR	April 9-10, 2008 (DC)	8 labs, 2 universities (counting NCAR)
Design and Testing of a Global Cloud-Resolving Model	D Randall, Colo State U	Project '11, SAP 09	BER (Lead), ASCR	April 9-10, 2008 (DC)	1 lab, 2 universities
Hybrid….Simulations of Subsurface Biogeochemical Processes	T. Scheibe, PNNL	Project '10, SAP 09	BER (Lead), ASCR	TBD	3 labs, 1 university
Modeling …... Subsurface Reactive Flows using Advanced Computing	P Lichtner, LANL	ends '11 - review early	BER (Lead), ASCR	TBD	4 labs, 1 university
National Computational Infrastructure for Lattice Gauge Theory	R Sugar, UC SantaBarbara	ends '11	HEP(lead), NP, ASCR	Jan, 2009 (DC)	3 labs, 10 universities
ComPASS (Accelerator Modelling)	P Spentzouris, FNAL	ends '11	HEP(lead), NP, BES, ASCR	March, 2009	6 labs, 3 universities, 1 industry
Quantum Simulations of Material and Nanostructures (Q-SIMAN)	G Galli, UC Davis	ends '11	NNSA(lead) ,ASCR	TBD	1 lab, 5 universities

ASCAC: October 28-29, 2008