Scientific Discovery through Advanced Computing

-- Update --

Presented to the

Advanced Scientific Computing Advisory Committee

Walter M. Polansky

Major Events

- **New SciDAC awards**
  - **Accelerator modeling and simulation**
  - **Computational biology**
- **FY2007 Continuing Resolution and Final Funding**
- **SciDAC Conference**
- **SciDAC Tutorial Workshop**
- **Committee of Visitors**

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

Challenges

Understand…
- materials properties; nano-scale through bulk
- gene function
- origin of dark energy
- subsurface transport phenomena
- behavior of ionized plasmas

…

Predict…
- materials performance under realistic conditions
- impact of human activities on climate
- migration of contaminants via groundwater
- fusion plasma behavior over extended time scales

…

Science Applications & Science Application Partnerships

Applied Math
Computer Science
Data Management
Visualization

INCITE
ESnet
Storage
NERSC
LCFs

Biology
Climate
Fusion Energy
Subsurface Flow
Materials & Chemistry
Physics

Centers for Enabling Technology & SciDAC Institutes

Direct Application Support

Education Outreach

Portability, Scaling, Performance, Analysis

Science Applications

Science Application Partnerships

Advanced Scientific Computing Research- SciDAC

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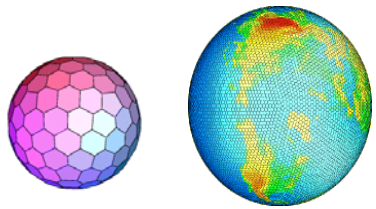
Global Climate Research including Role of Clouds

Petascale Communications for Open Science



Quantum Simulations and predictive modeling of materials and stress corrosion

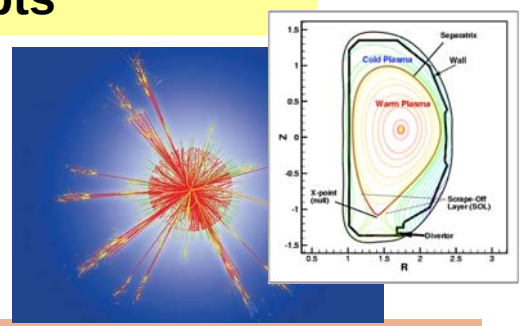
Building an Energy Density Function validated by existing data for predicting critical unknowns

Modeling for Accelerator Design including Beam Dynamics, Electromagnetics, and Advanced Accelerator concepts

Fusion Simulations towards Integrating Systems

Subsurface Flows and Biogeochemical Processes

Quarks on the Lattice and Exploding Supernovae



Turbulence and Shock Waves, Computational Chemistry & Life Sciences

Computational Biology Project

Advanced Scientific Computing Research- SciDAC

- **"Understanding the Processivity of Cellobiohydrolase Cel7A (CBH I)"**
  - **NREL, Michael Himmel - PI**
  - **ORNL,**
  - **Cornell University,**
  - **The Scripps Research Institute,**
  - **San Diego Supercomputer Center,**
  - **UC San Diego,**
  - **Forest Products Research Lab**

- Partnership between ASCR and BER.
- Directly aligned with the GTL long-term PART goal for both programs.
- Budget of about $1M/year for 5 years.

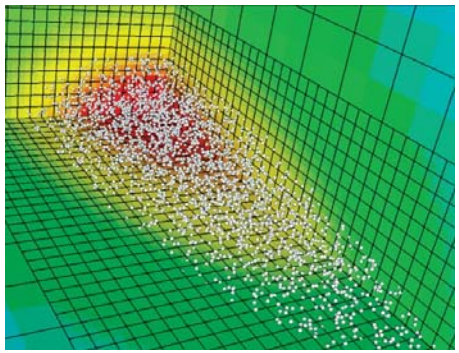
- **To investigate the mechanism of action of cellulose-degrading enzymes through a multidisciplinary collaboration that will use molecular dynamics (MD) simulations and to expand the capabilities of these MD codes to allow simulations of enzymes and substrates on peta-scale computational facilities.**
- **Improving efficiency of producing ethanol from lignocellulose- a vital step in reducing our nation's dependence on foreign oil.**
- **This project could provide fundamental advances in our understanding of the action of critically important microbial systems and cellulose degrading enzymes acting on cellulose.**

U.S. Department of Energy

Office of Science

Community Petascale Project for Accelerator Science and Simulation (COMPASS)

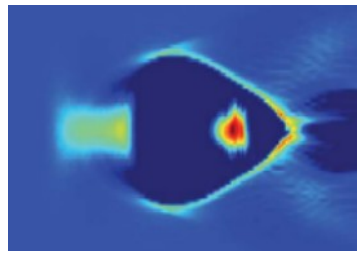
Advanced Scientific Computing Research- SciDAC



Terascale to the Petascale

Computational and Modeling Studies for Accelerator Design Research

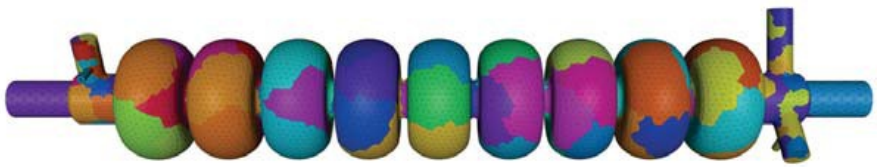
Beam Dynamics, Electromagnetics, and Advanced Accelerator Concepts



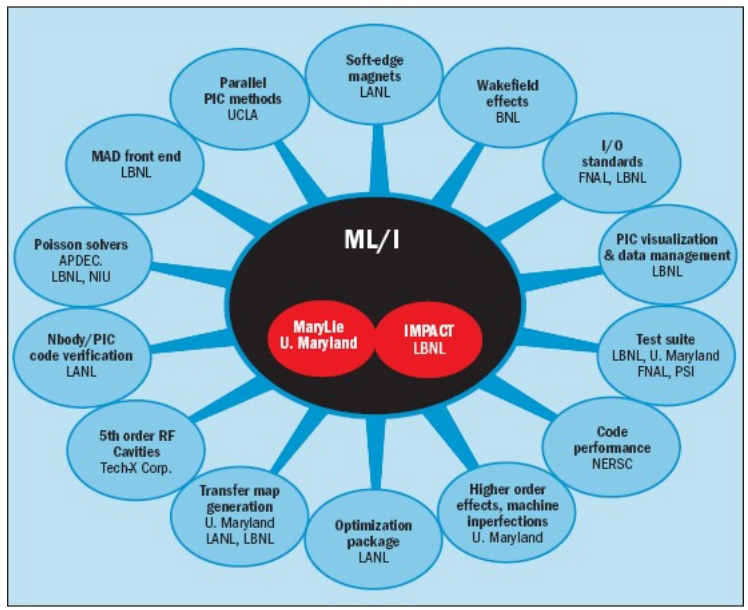
$3M/yr. project; (ASCR- $500K/yr)

PI: Panagiotis Spentzouris

Collaborating Institutions: FNAL(lead), ANL, BNL, LBNL, LANL, ORNL, SLAC,Stonybrook U, TechX, TJNAL, U. Cal. Davis, U. Cal. LA, UMD.



Applications for LHC, ILC, CeBAF, SNS….

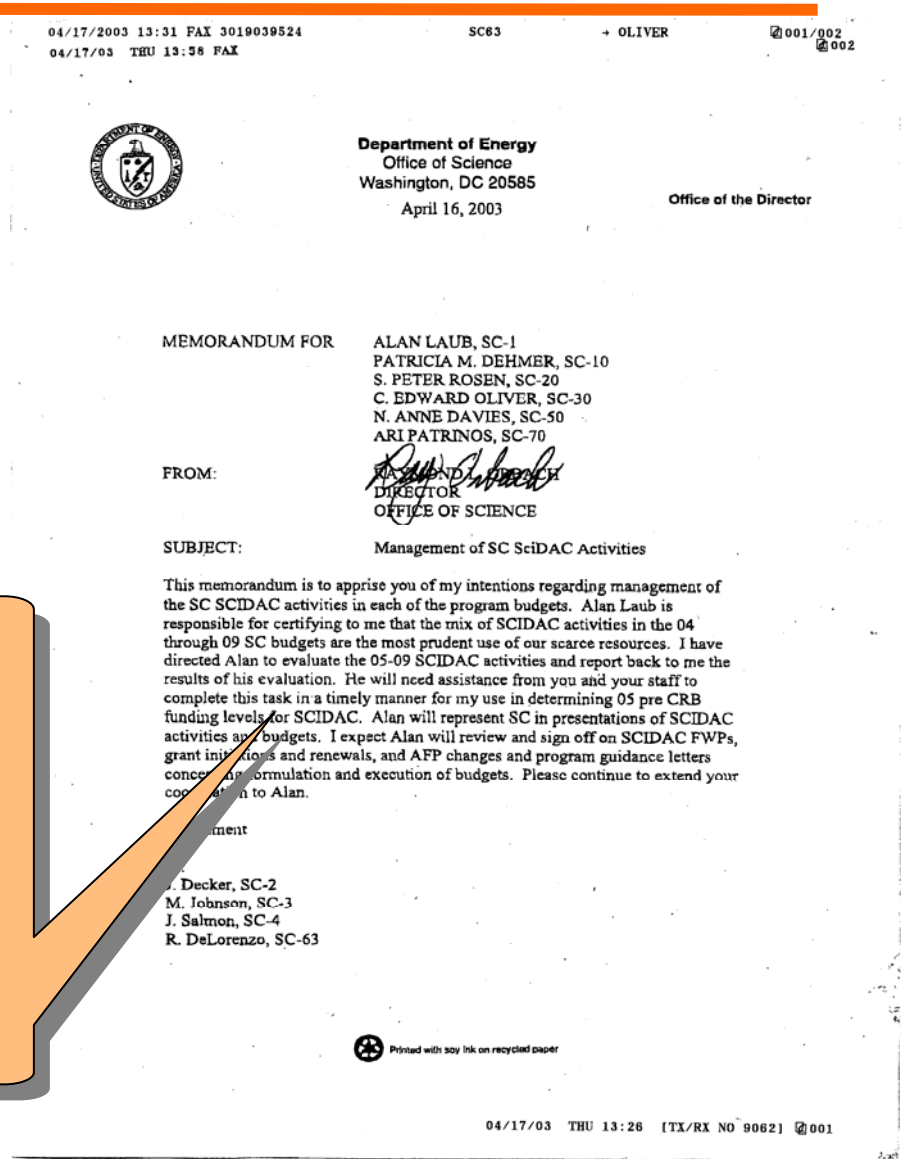


SciDAC Management Policy

-- 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."



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04/17/03 THU 13:58 FAX 002

Department of Energy
Office of Science
Washington, DC 20585
April 16, 2003

Office of the Director

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.

...ment

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

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SciDAC-2 Coordinating Group

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

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

SciDAC Centers

Title	Lead PI	Lead Institution	Partners	
			Univ	Labs
Center for Technology for Advanced Scientific Component Software	BERNHOLDT	ORNL	5	6
Visualization and Analytics Center for Enabling Technologies (CET)	BETHEL	LBNL	2	4
APDEC: The Applied Partial Differential Equations CET	COLELLA	LBNL	1	3
Center for Enabling Distributed Petascale Science	FOSTER	ANL	2	3
Center for Interoperable Technologies for Advanced Petascale Simulations (ITAPS)	FREITAG-DIACHIN	LLNL	3	5
Institute for Scalable-Performance Application Development Software	MELLOR-CRUMMEY	Rice University	4	1
Towards Optimal Petascale Simulations (TOPS)	KEYES	Columbia University	5	4
Scientific Data Management	SHOSHANI	LBNL	5	5
Scaling the Earth System Grid to Petascale Data	WILLIAMS	LLNL	3	5

SciDAC Institutes

Title	Lead PI	Lead Institution	Partners	
			Univ	Labs
Petascale Data Storage Institute	GIBSON	Carnegie Mellon Univ.	UC Santa Cruz, Michigan	LBNL, LANL, ORNL, PNNL, SNLA
Performance Engineering Research Center for Enabling Technologies	LUCAS	University of Southern California	Rice, UC San Diego, Univ. Southern Cal, Maryland, North Carolina, Tennessee	ANL, LBNL, LLNL, ORNL
Ultrascale Visualization	MA	University of California at Davis	Ohio State, Tennessee, Virginia	ANL, SNLA
Combinatorial Scientific Computing and Petascale Simulations (CSCAPES)	POTHEN	Old Dominion University	Ohio State	ANL, SNLA

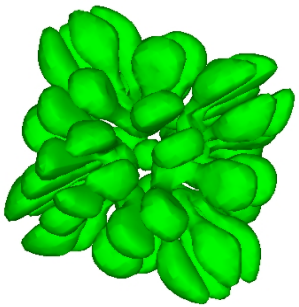
FY2007 Funding Resolution Impacts

- **Centers for Enabling Technology**
  - **5 university partners (20%) placed on 90 day no-fund extension**
- **Institutes**
  - **15 university partners (95%) placed on 90-day no-fund extension**
- **Science Application Partnership**
  - **1 placed on 90-day no-fund extension**

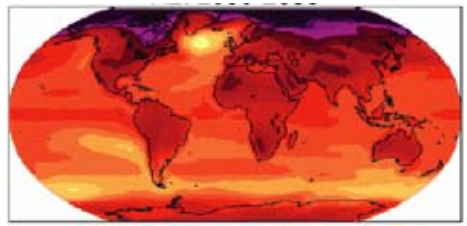
SciDAC 2007

Office of Science

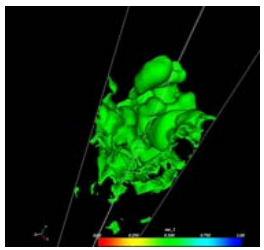
Scientific Discovery through Advanced Computing
June 24 - 28 Boston

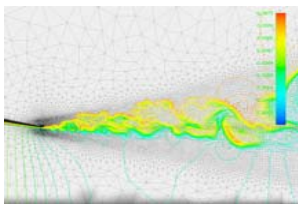


SciDAC Conference

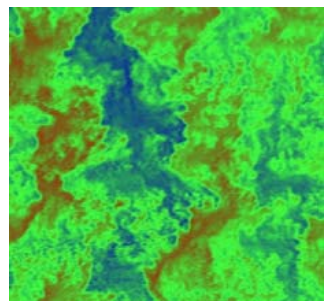


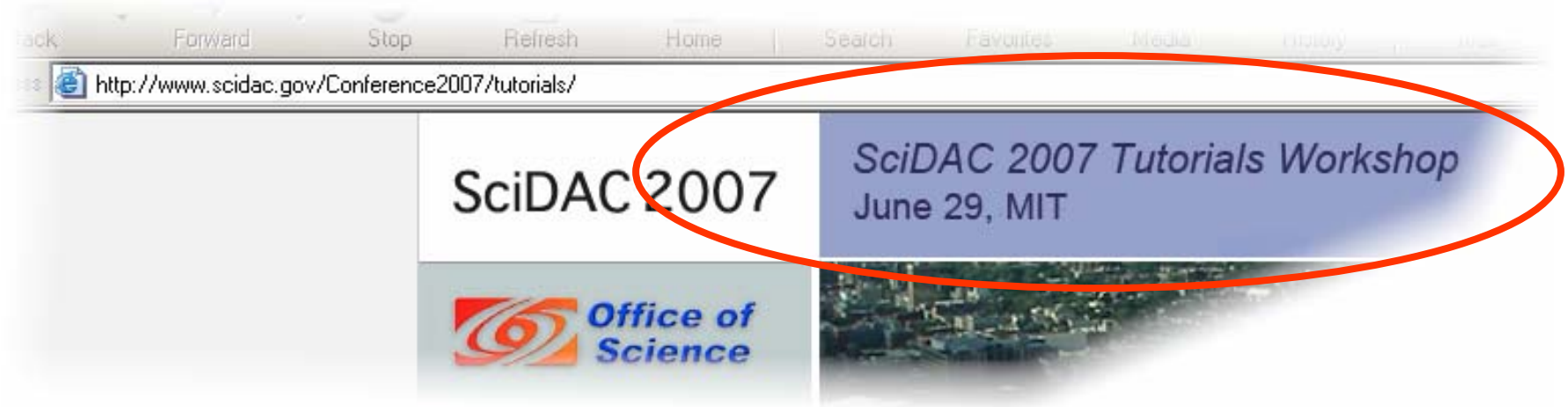
- **Registered participants- over 300 (55 universities, 20 national laboratories, 14 private companies, 5 government agencies and 4 countries)**
- **Plenary talks- 36**
- **Posters- 76**
- **Panels- 2**





http://www.scidac.gov/Conference2007/





- **Theme: An introduction to using SciDAC software**
- **Tutorials offered by 3 SciDAC applications, 6 Centers; 1 Institute**
- **Lectures and live runs on local Blue/Gene L**
- **115 participants (many post-docs and graduate students)**

Sponsors:

- **The Laboratory for Nuclear Science, Massachusetts Institute of Technology**
- **CyberInfrastructure Engineering Lab, Harvard School of Engineering & Applied Sciences**
- **Center for Computational Science, Boston University**
- **SciDAC Outreach Center**

Recognitions & Accomplishments

Advanced Scientific Computing Research- SciDAC

Dean Williams (LLNL), PI of Earth System Grid CET, received an Emerald Award, a premier award for African Americans, Hispanics, Asian Americans and Native Americans working in the research sciences.

William Gropp, (ANL) a senior researcher in SDM CET, named fellow of the Association for Computing Machinery (ACM).

CSCAPES researchers (U.V. Catalyurek, E.G. Boman, K.D. Devine, D. Bozdag, R. Heaphy, L.A. Riesen) awarded best paper in Algorithms at IEEE Conference- 2007

CScADS convened 4 workshops to familiarize the community with the challenges of DOE petascale systems, and provide interfaces between tool developers and application developers.

Center for Scalable Application Development Software

SciDAC Outreach Center

A pilot program to establish a central resource for inquiries and technical information about SciDAC.

- **Major activities**
  - **Helping SciDAC projects organize/develop/update/test software (major interactions with VACET, PERI, OSG & UNEDF)**
  - **Responding to inquiries (43 so far)**
- **Plans**
  - **Develop portal services**
  - **Expand outreach services to industry**
  - **Prepare for peer review**