Office of Science
Science for America's Future

The Launch of Scientific Discovery through Advanced Computing

Presentation to Advanced Scientific Computing Advisory Committee

Washington, DC

October 25-26, 2001

Stephen Eckstrand
Former Director, SciDAC

http://www.science.doe.gov/SciDAC/

SciDAC Goals

An **integrated** program to:

(1) Create a new generation of Scientific Simulation Codes that take full advantage of the extraordinary computing capabilities of terascale computers.

(2) Create the Mathematical and Computing Systems Software to enable these Scientific Simulation Codes to use terascale computers effectively and efficiently .

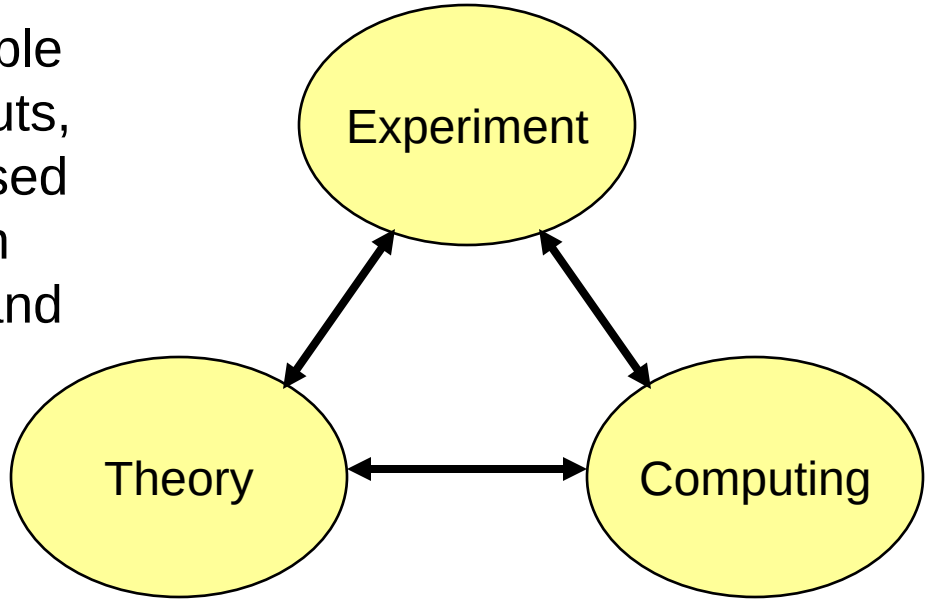
(3) Create a Collaboratory Software Environment to enable geographically separated scientists to work together as an integrated team and to facilitate remote access to both facilities and data.

SciDAC Vision

SciDAC-Integrating Science and Computing

Just within the past few years, advanced scientific computing has reached a point where it is on a par with laboratory experiment and mathematical theory as a major tool for scientific discovery.

Major increases in computing power will enable a new generation of simulation codes, based on reliable experimental and theoretical inputs, to lead the way to greatly increased scientific understanding, which in turn will lead to new theoretical and experimental discoveries.



Program Management Strategies

- Development of next generation modeling and simulation codes, mathematical algorithms, systems software, along with computing and network resource planning are interdependent activities that must be carefully managed.
  - Coordinate planning and management of SciDAC activities across the Office of Science (SciDAC director and a SciDAC Coordinating Committee)
  - Establish integrated scientific challenge teams (applications scientists, applied mathematicians, and computer scientists) with clear deliverables
  - Provide reliable access to adequate supercomputing and network resources

SciDAC Coordinating Committee

SciDAC-Integrating Science and Computing

- Dave Bader, BER
- Bill Kirchhoff, BES
- Walter Stevens, BES
- Steve Eckstrand, FES
- Arnold Kritz, FES
- Robin Staffin, HENP
- Vicky White, HENP
- Fred Johnson, ASCR
- Buff Miner, ASCR
- Thomas Ndousse, ASCR
- Kimberly Rasar, ASCR
- Chuck Romine, ASCR
- Mary Anne Scott, ASCR
- George Seweryniak, ASCR

SciDAC Program History

- Develop SciDAC Strategic Plan 3/2000
- Prepare Budget Requests 1999-2000
- Prepare Solicitations (6) 12/2000
- Conduct Merit Reviews 4-5/2001
- Make Funding Recommendations 6/2001
- Prepare Grant and Contract Awards 6-7/2001
- Manage Start of Individual Projects 7-9/2001
- Prepare for PI Meeting 10-12/2001

Initial Awards Focus on Software

SciDAC-Integrating Science and Computing

- **Scientific Applications**
  - Climate Simulation
  - Computational Chemistry
  - Fusion – 5 topics
  - High Energy/Nuclear Physics – 5 topics
- **Collaboratories**
  - Four projects
- **Middleware & Network Research**
  - Six projects
- **Computer Science**
  - Scalable Systems Software
  - Common Component Architecture
  - Performance Science and Engineering
  - Scientific Data Management
- **Applied Mathematics**
  - PDE Linear/Nonlinear Solvers and Libraries
  - Structured Grids/AMR
  - Unstructured Grids

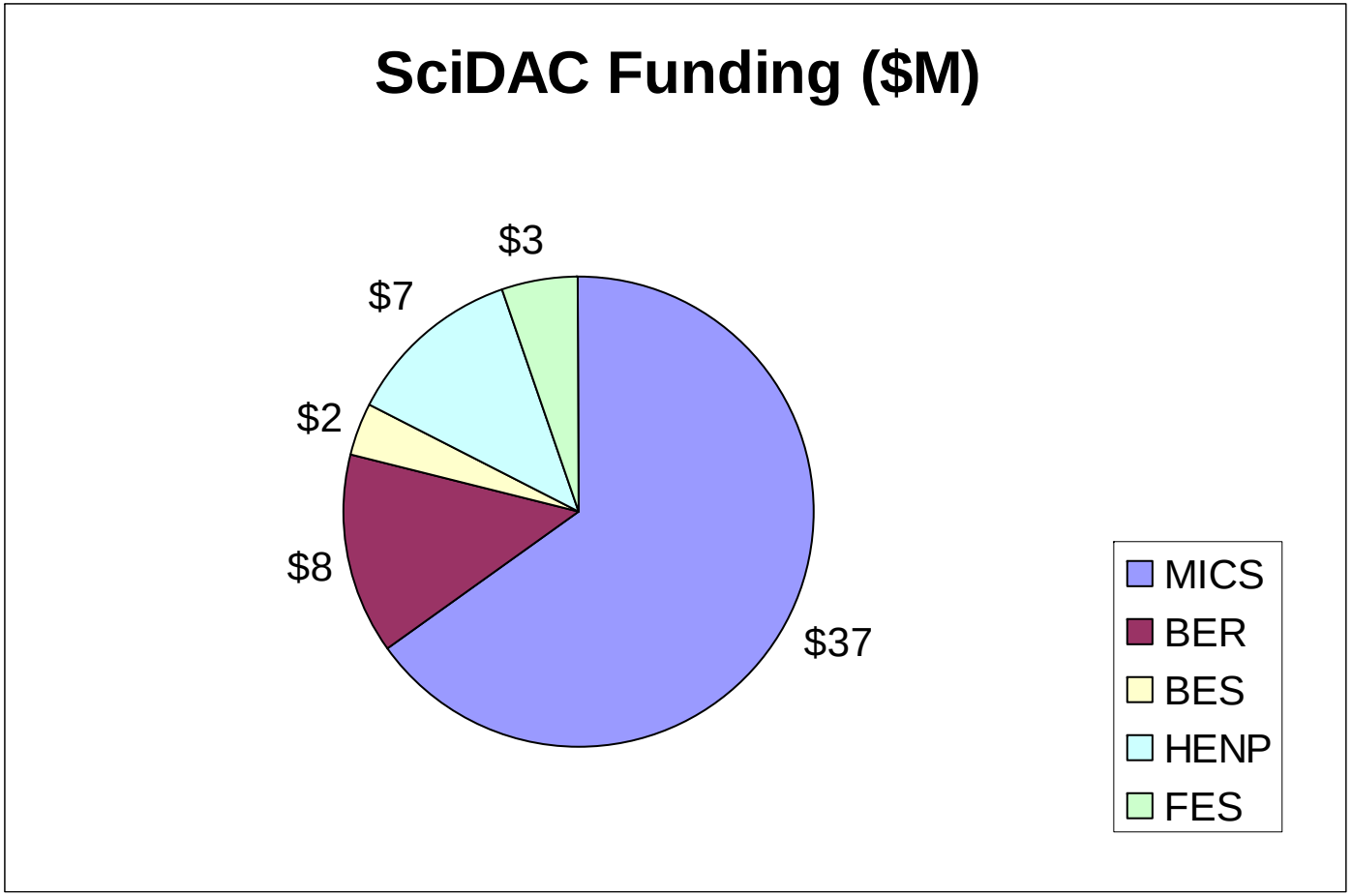
Initial Awards Support Teams

SciDAC-Integrating Science and Computing

Twenty-four projects funded at $500K-$3M per year

First Year Funding Distribution

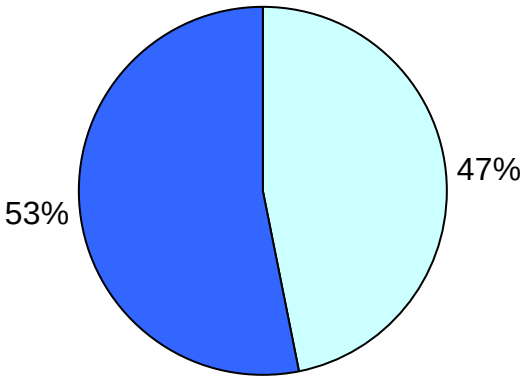
SciDAC-Integrating Science and Computing



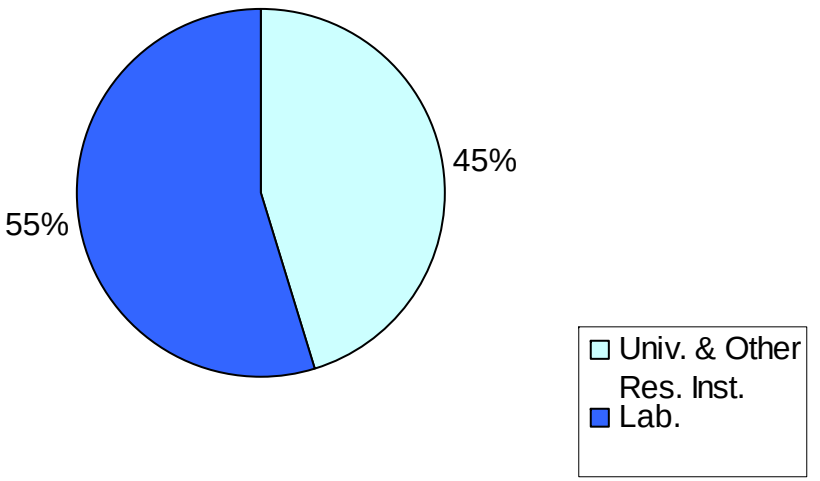
Distribution of Funding between National Labs and Universities

SciDAC-Integrating Science and Computing

SciDAC - MICS Awards: $37M



SciDAC - Total Awards: $57M



Thirteen National Labs Involved

SciDAC-Integrating Science and Computing

- Ames Laboratory
- Argonne National Laboratory
- Brookhaven National Laboratory
- Fermi National Accelerator Laboratory
- Lawrence Berkeley National Laboratory
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- Oak Ridge National Laboratory
- Pacific Northwest National Laboratory
- Princeton Plasma Physics Laboratory
- Thomas Jefferson Laboratory
- Sandia National Laboratory
- Stanford Linear Accelerator

Fifty-three Universities in 26 States and Province of Quebec Involved

SciDAC-Integrating Science and Computing

Auburn University; Boston University; California Institute of Technology; Carnegie Mellon University; Clemson University; Colorado State University; Florida Atlantic University; Georgia Institute of Technology; Indiana University; Iowa State University; Massachusetts Institute of Technology; Michigan State University; New York University; North Carolina State University; Northwestern University; Ohio State University; Oklahoma State University; Old Dominion University; Princeton University; Rensselaer Polytechnic Institute; Rice University; Rollins College; Rutgers University; Scripps Institute (UCSD); Stanford University; State University New York at Stony Brook; Stevens Institute of Technology; University Corporation for Atmospheric Research; University of Arizona; University of California Berkeley; University of California Davis; University of California Los Angeles; University of California San Diego; University of California Santa Barbara; University of California Santa Cruz; University of Chicago; University of Colorado; University of Delaware; University of Georgia; University of Illinois at Urbana-Champaign; University of Iowa; University of Maryland; University of Michigan; University of North Carolina; University of Quebec (Canada); University of Southern California; University of Tennessee; University of Texas at Austin; University of Utah; University of Washington; University of Wisconsin - Madison; Utah State University; and Wellesley College

Computational Chemistry Awards

SciDAC-Integrating Science and Computing

Two Projects on modeling of combustion, one project on heavy element chemistry, and eight projects on chemical structures and reactivity - $1.9M

Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry	Sandia National Laboratory (Habib Najm, SNL)	$300K/Yr
Reliable Electronic Structure Calculations for Heavy Element Chemistry: Molecules Containing Actinides, Lanthanides, and Transition Metals	Arnaud Trouve, Univ. of Maryland Hong Geun Im, Univ. of Michigan Christopher J. Rutland, Univ. of Wisconsin-Madison	$227K/Yr
Reliable Electronic Structure Calculations for Heavy Element Chemistry: Molecules Containing Actinides, Lanthanides, and Transition Metals	Walter Ermler, Stevens Institute Russ Pitzer, Ohio State Univ.	$198K/Yr

Computational Chemistry (Continued)

SciDAC-Integrating Science and Computing

Advanced Methods for Electronic Structure	Robert Harrison, PNNL Martin Head-Gordon, LBNL	$375K/Yr
Advancing Multi-Reference Methods in Electronic Structure Theory	Mark S. Gordon, Ames Laboratory	$250K/Yr
New Coupled-Cluster Methods for Molecular Potential Energy Surfaces	Piotr Piecuch, Michigan State	$110K/Yr
Accurate Properties for Open-Shell States of Large Molecules	Peter Taylor, UCSD	$121K/Yr
Explicitly Correlated Coupled Cluster & Bruecker Methods for Computations of Properties of Chemical Accuracy for Open Shell Systems	Fritz Schaefer, Univ. of Georgia	$66K/Yr
Linear Scaling electronic Structure Methods with Periodic Boundary Conditions	Gustavo E. Scuseria, Rice Univ.	$100K/Yr
Advanced Software for the Calculation of Thermochemistry, Kinetics and Dynamics	Albert F. Wagner, Argonne National Laboratory	$85K/Yr
Theoretical Chemical Dynamics Studies of Elementary Combustion Reactions	Donald L. Thompson, Oklahoma State Univ.	$95K/Yr

Combustion

SciDAC-Integrating Science and Computing

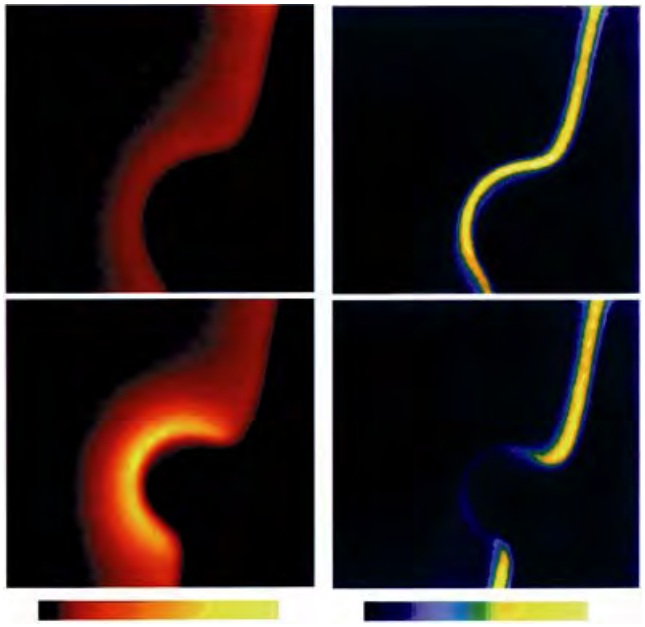
Models for predicting combustion processes including full chemistry and the interaction of chemistry with fluid dynamics

Participants …

Sandia National Laboratories

University of Maryland
University of Michigan
University of Wisconsin

Laser induced fluorescence imaging of the interaction of chemistry with fluid dynamics Profiles of species CH and OH with time



3 millisec after vortex reaches flame surface

5 millisec after vortex reaches flame surface

Predicting Molecular Structure and Reactivity

SciDAC-Integrating Science and Computing

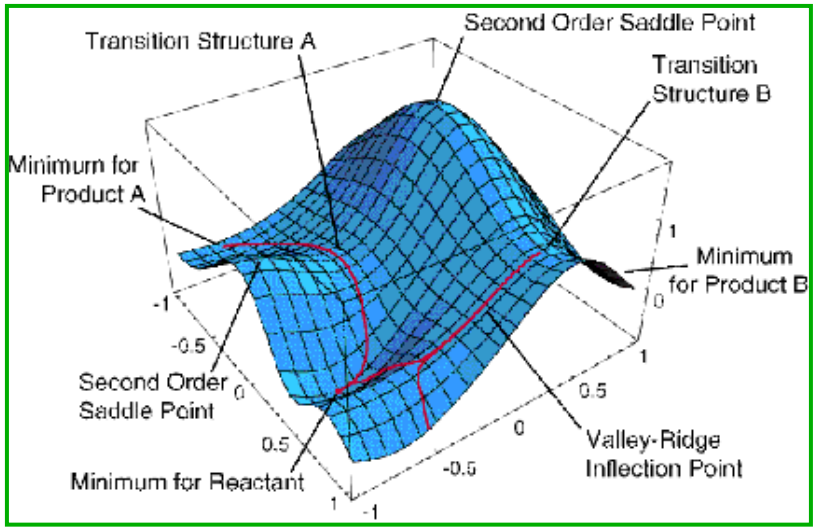
Chemically accurate calculations of the properties of molecules with with an emphasis on excited states and reactive radicals important in combustion

Participants …

Pacific Northwest National Laboratory
Lawrence Berkeley National Laboratory
Argonne National Laboratory
Ames Laboratory

Michigan State University
University of California, San Diego
University of Georgia
Rice University
Oklahoma State University

A potential energy surface, showing regions of importance in modeling structure and reactivity



Modeling Heavy Element Chemistry

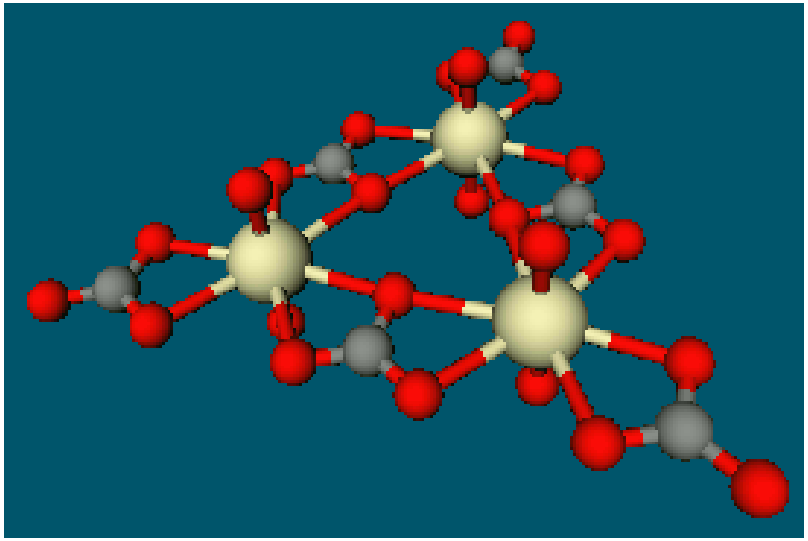
SciDAC-Integrating Science and Computing

Calculation of properties of lanthanide and actinide compounds for which experiments are impractical and to aid in the interpretation of experiments

Participants …

Pacific Northwest National Laboratory

Stevens Institute of Technology
Ohio State University



Uranium Carbonate Complex
$(UO_2)_3(CO_3)_6$

Fusion Energy Sciences Awards

SciDAC-Integrating Science and Computing

Five Projects to develop key elements of an integrated model for the simulation of fusion plasma systems - $3.0M

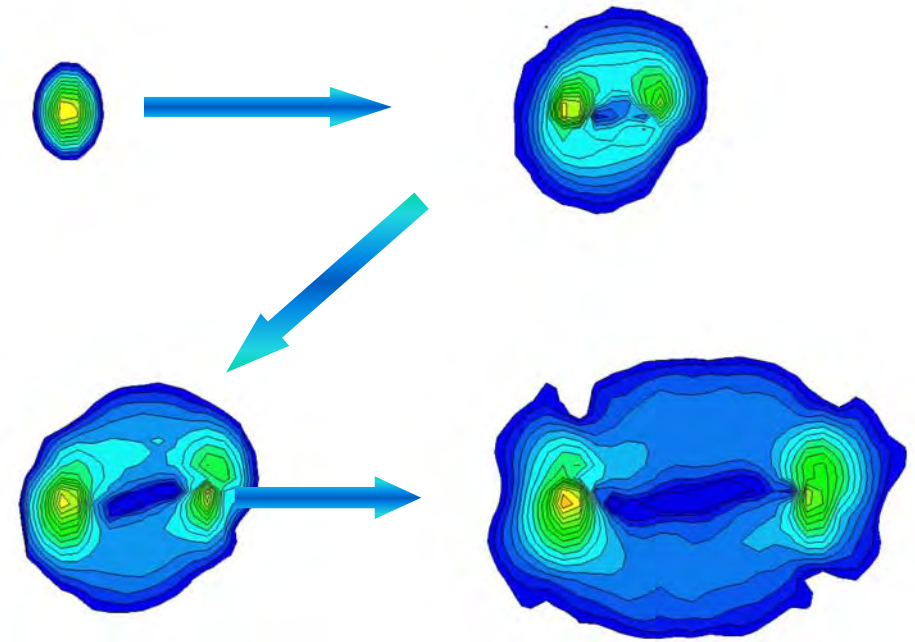
Magnetic Reconnection: Applications to Sawtooth Oscillations, Error Field Induced Islands & the Dynamo Effect	Univ. Of Iowa Univ. of Chicago Univ. of Texas (Amitava Bhattacharjee, Univ. of Iowa)	$750K/Yr
Terascale Computational Atomic Physics for the Edge Region in Controlled Fusion Plasmas	Auburn Univ. Rollins Coll. ORNL (Mitch Pindzola, Auburn)	$300K/Yr
Numerical Computation of Wave-Plasma Interactions in Multi-dimensional Systems	ORNL PPPL MIT Lodestar CompX (Don Batchelor, ORNL)	$1.0M/Yr
Center for Extended MHD Modeling	PPPL SAIC MIT Utah State Univ. Univ. of Wisconsin Univ. of Colorado NYU (Steve Jardin, PPPL)	$500K/Yr
Plasma Microturbulence Project	LLNL PPPL UCLA Univ. of Maryland General Atomics Univ. of Colorado (Bill Nevins, LLNL)	$450K/Yr

Fusion Energy Sciences Projects

SciDAC-Integrating Science and Computing

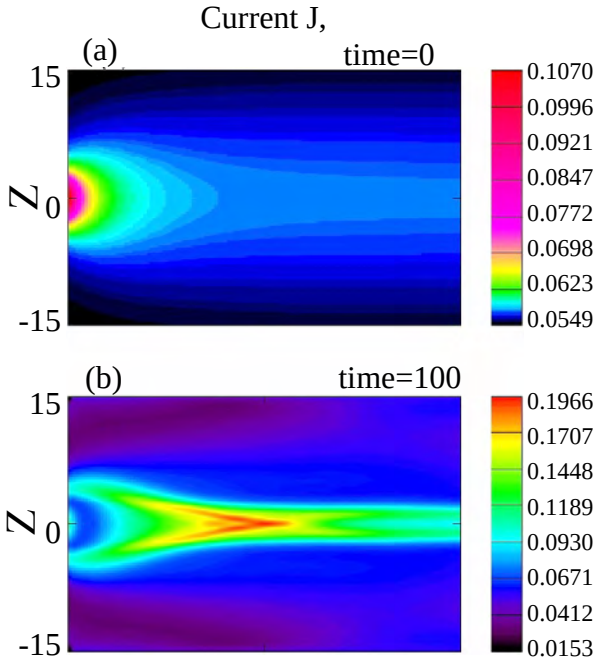
Terascale Atomic Physics

Auburn University
Rollins College
Oak Ridge National Laboratory



Electron Probability Distribution during Atom-Molecule Collision

Substorm in the Magnetotail



Magnetic Reconnection Code

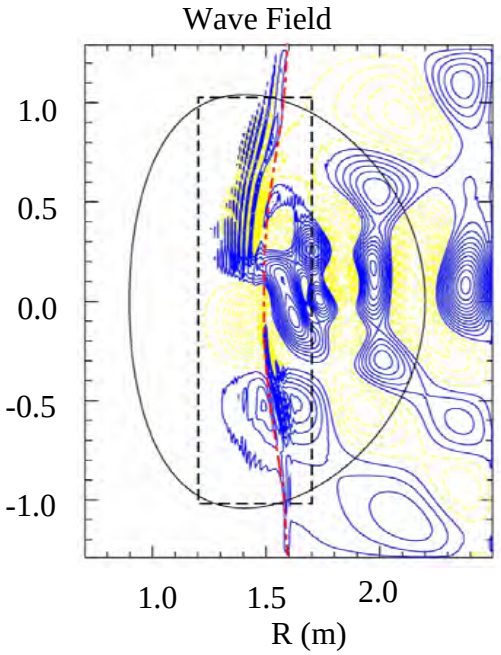
University of Iowa
University of Chicago
University of Texas

Fusion Energy Sciences Projects

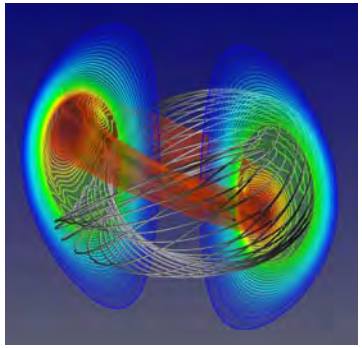
SciDAC-Integrating Science and Computing

Computation of Wave Plasma Interactions

ORNL, PPPL, MIT, Lodestar, CompX



Extended MHD Modeling

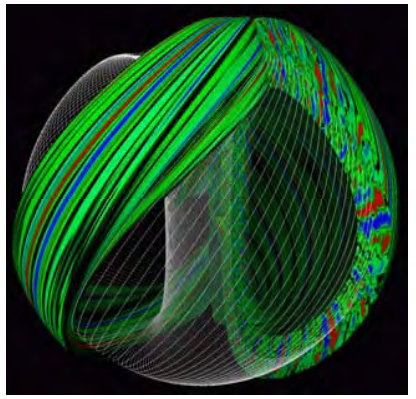


PPPL, SAIC, U. Wisconsin, NYU, U. Colorado, MIT, Utah State U., GA, LANL, U. Texas

M=1, N=1 Plasma Instability

Plasma Microturbulence

LLNL, GA, PPPL, U. Maryland, U. Texas, U. Colorado, UCLA



Turbulent Eddies in Plasma

High Energy/Nuclear Physics Awards

SciDAC-Integrating Science and Computing

Four Scientific Simulation project awards were made and one Collaborative Pilot award (jointly with ASCR) for a total of $6.9M of HENP funding

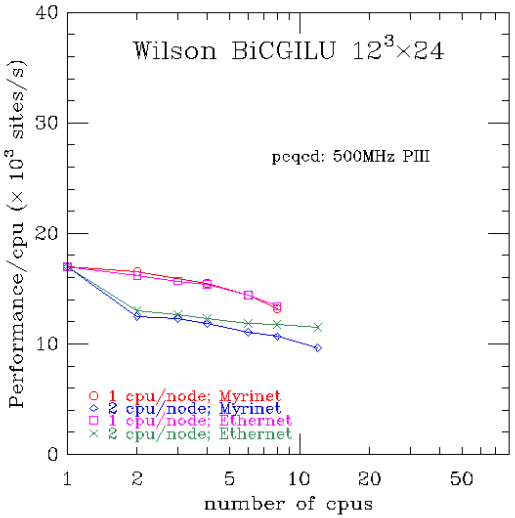
National Computational Infrastructure for Lattice Gauge Theory	UCSB BU MIT Columbia FNAL BNL TJNAF U. Arizona U. Utah UIUC	$1.86M/Yr
Advanced Computing for 21st Century Accelerator Science and Technology	LBNL SLAC FNAL SNL UCLA Stanford U. Maryland U. Southern California UC Davis Tech-X Corp.	$1.8 M/Yr
Shedding New Light on Exploding Stars: Terascale Simulations of Neutrino-Driven Supernovae and Their Nucleosynthesis	ORNL U. Illinois U. Tennessee N.C. State U. Florida Atlantic U. Clemson U. UC San Diego	$1.25M/Yr
SciDAC Center of Supernova Research	UC Santa Cruz U. Arizona LANL LLNL	$0.52M/Yr
Particle Physics Data Grid Collaborative Pilot	Univ. of Wisconsin UCSD Caltech BNL FNAL ANL JLAB LBNL SLAC	$1.44M/Yr (Joint with ASCR)

High Energy and Nuclear Physics Projects

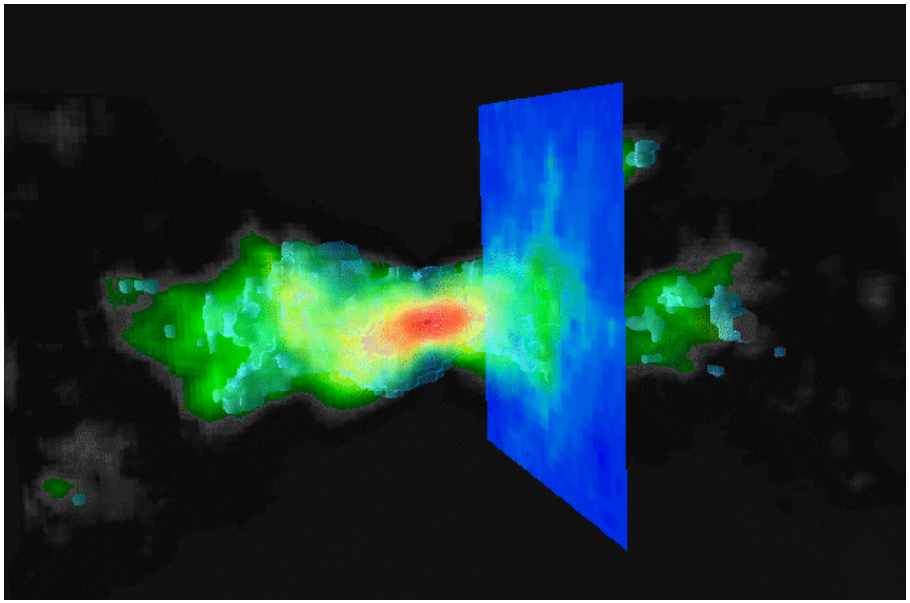
SciDAC-Integrating Science and Computing

National Computational Infrastructure For Lattice Gauge Theory (Sugar)

Representing ~60 theorists in the US.
Funding to 3 labs and 6 universities



Analysis of calculation on Lattice



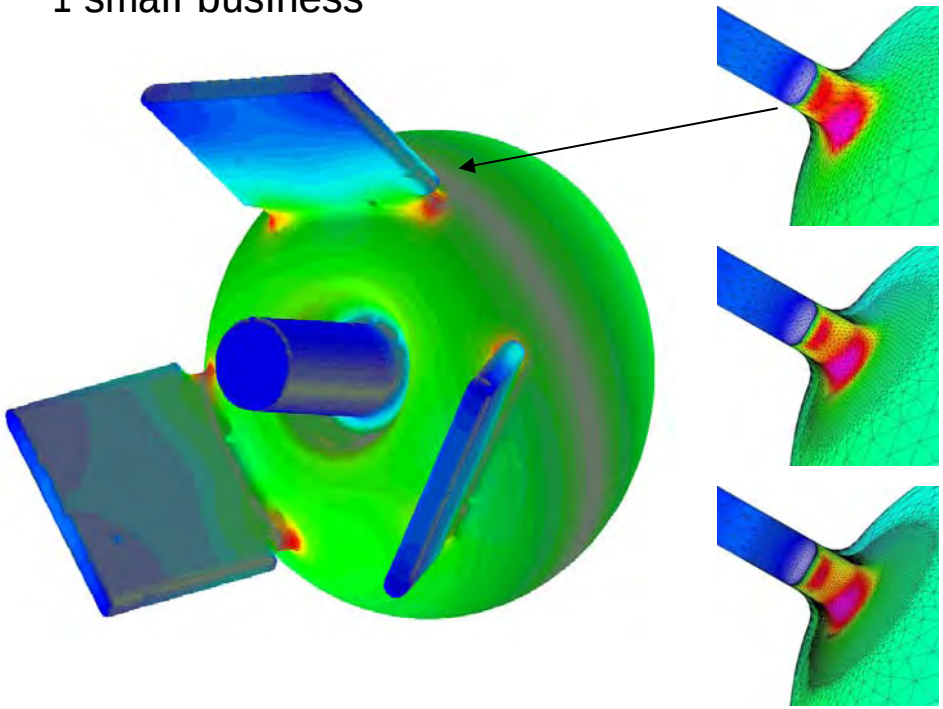
Quark propagator

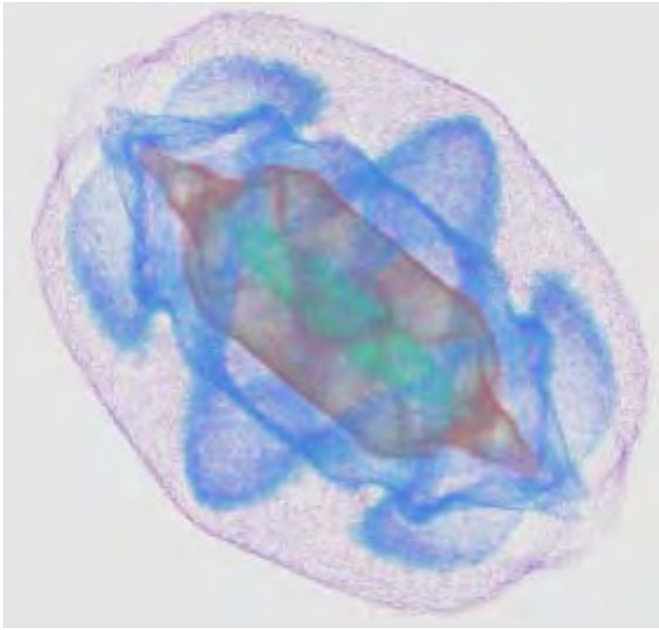
High Energy and Nuclear Physics Projects

SciDAC-Integrating Science and Computing

Advanced Computing for 21st Century Accelerator Science and Technology(Ryne, Ko)

Funding to 4 labs, 4 universities and 1 small business





Simulation of intense beam exhibits ultra-low density beam halo

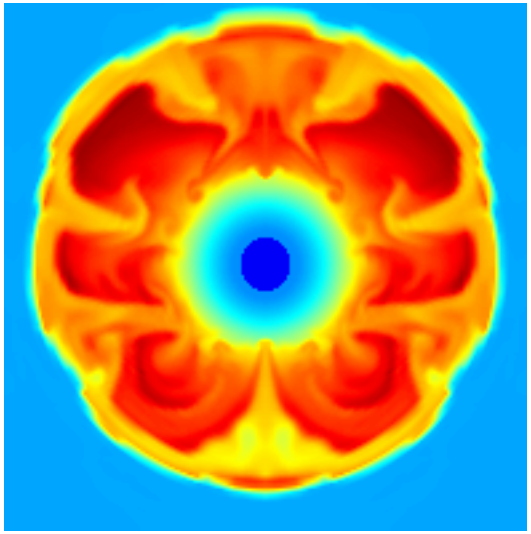
Simulation provides high resolution needed to predict peak power loss in complex electromagnetic cavity

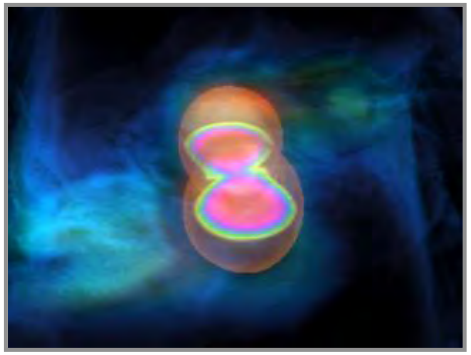
High Energy and Nuclear Physics Projects

SciDAC-Integrating Science and Computing

Shedding New Light on Exploding Stars: Terascale Simulations of Neutrino-Driven Supernovae and their Nucleosynthesis
(Mezzacappa)

Funding to 1 lab and 8 universities





Problem: How to reveal local features occurring in a larger structure?
Build customized RenderMan *data shaders.*

Instrumented 3D hydrodynamics code monitored using CUMULUS

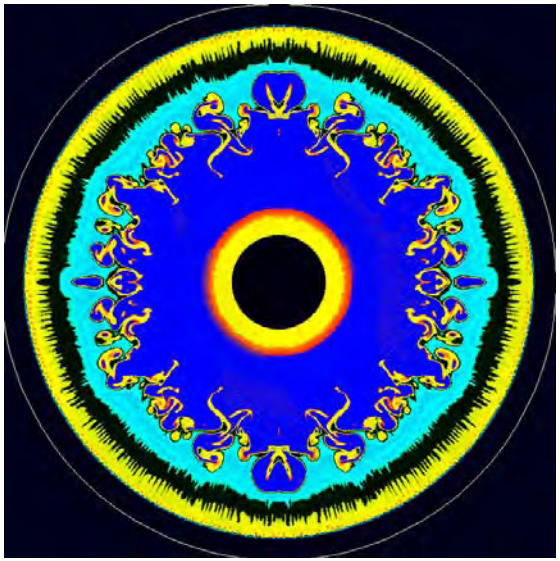
High Energy and Nuclear Physics Projects

SciDAC-Integrating Science and Computing

SciDAC Center for Supernova Research (Woosley)

Funding to 2 labs and 2 universities

Impact of a supernova on an adjacent star



Protoneutron star convection

High Energy and Nuclear Physics Projects

SciDAC-Integrating Science and Computing

The Particle Physics Datagrid Collaboratory Pilot
(Mount, Newman, Livny)

Jointly funded with ASCR

Funding to 6 labs and 3 universities

Involves major HEP and NP experiments

Babar, DO, CMS, ATLAS, STAR

Climate Modeling Awards

SciDAC-Integrating Science and Computing

Two large projects to develop a community climate model and the climate model of the future; 13 smaller projects to develop advanced climate model elements - $7.9M

Collaborative Design and Development of the Community Climate System Model for Terascale Computers	ORNL LBNL PNNL ANL LLNL NCAR (Robert Malone, LANL)	$4.0M/Yr
A Geodesic Climate Model with Quasi-Lagrangian Vertical Coordinates	LANL Clarkson Univ. (David Randall, Colorado State Univ.)	$802K/Yr
Predictive Understanding of the Oceans' Wind-Driven Circulation on Interdecadal Time Scales	Indiana Univ. (Michael Ghil, UCLA)	$192K/Yr
Decadal Variability in the Coupled Ocean-Atmosphere Systems	(Paola Cessi, UCSD)	$155K/Yr
Improving the Processes of Land-Atmosphere Interactions in CCSM 2.0 at High Resolution	University of Arizona (Robert Dickinson, Georgia Tech)	$245K/Yr
Continuous Dynamic Grid Adaptation in a Global Atmospheric Model	(William Gutowski, Iowa State Univ.)	$148K/Yr

Climate Modeling Awards (Continued)

SciDAC-Integrating Science and Computing

Decadal Regional Climate Studies and Applications with Variable-Resolution GCMs Using Advanced Numerical Techniques	(Michael Fox-Rabinovitz, Univ. of Maryland)	$228K/Yr
Multi-Resolution Climate Modeling	(Ferdinand Baer, Univ. of Maryland)	$180K/Yr
Development of an Atmospheric Climate Model with Self-Adapting Grid and Physics	(Joyce Penner, Univ. of Michigan)	$270K/Yr
Testing a New Hybrid Ocean Circulation Model Based on POP	LANL (Kirk Bryan, Princeton Univ.)	$87K/Yr
Decadal Regional Climate Studies and Applications with Variable-Resolution GCMs Using Advanced Numerical Techniques	(Jean Cote, Univ. of Quebec)	$69K/Yr
Modeling Dynamic Vegetation for Decadal to Multi-Century Climate Change Studies	Goddard Institute for Space Sci. (Andrew Friend, Rutgers Univ.)	$72K/Yr

Climate Modeling Awards (Continued)

SciDAC-Integrating Science and Computing

Towards the Prediction of Decadal to Multi-Century Processes in a High-Throughput Climate System Model	(Zhengyu Liu, Univ. of Wisconsin) (John Kutzbach, Univ. of Wisconsin)	$231K/Yr
Modeling and Analysis of Global and Regional Hydrologic Processes and Appropriate Conservation of Moist Entropy	(Donald Johnson, Univ. of Wisconsin)	$231K/Yr

Collaboratory Awards

SciDAC-Integrating Science and Computing

Three Pilot Collaboratories and One Services Infrastructure Pilot to develop and demonstrate software that allows distributed teams to work together effectively and access data and facilities remotely - $8.7M

A National Collaboratory to Advance the Science of High Temperature Plasma Physics for Magnetic Fusion	Princeton Univ. Univ. of Utah LBNL PPPL ANL (David Schissel, General Atomics)	$1.8M/Yr
Particle Physics Data Grid Collaborative Pilot	Univ. of Wisc. UCSD Cal Tech BNL Jlab SLAC ANL LBNL (Ruth Pordes, FNAL)	$3.19M/Yr (Joint with HENP)
Earth Systems Grid II: Turning Climate Datasets into Community Resources	UCAR ORNL LLNL (Don Middleton, UCAR)	$1.82M/Yr
DOE Science Grid: Enabling and Deploying the SciDAC Collaboratory Software Environment	ANL PNNL ORNL (Bill Johnston, LBNL)	$1.88M/Yr

The Vision for a DOE Science Grid

Scientific applications use workflow frameworks to coordinate resources and solve complex, multi-disciplinary problems

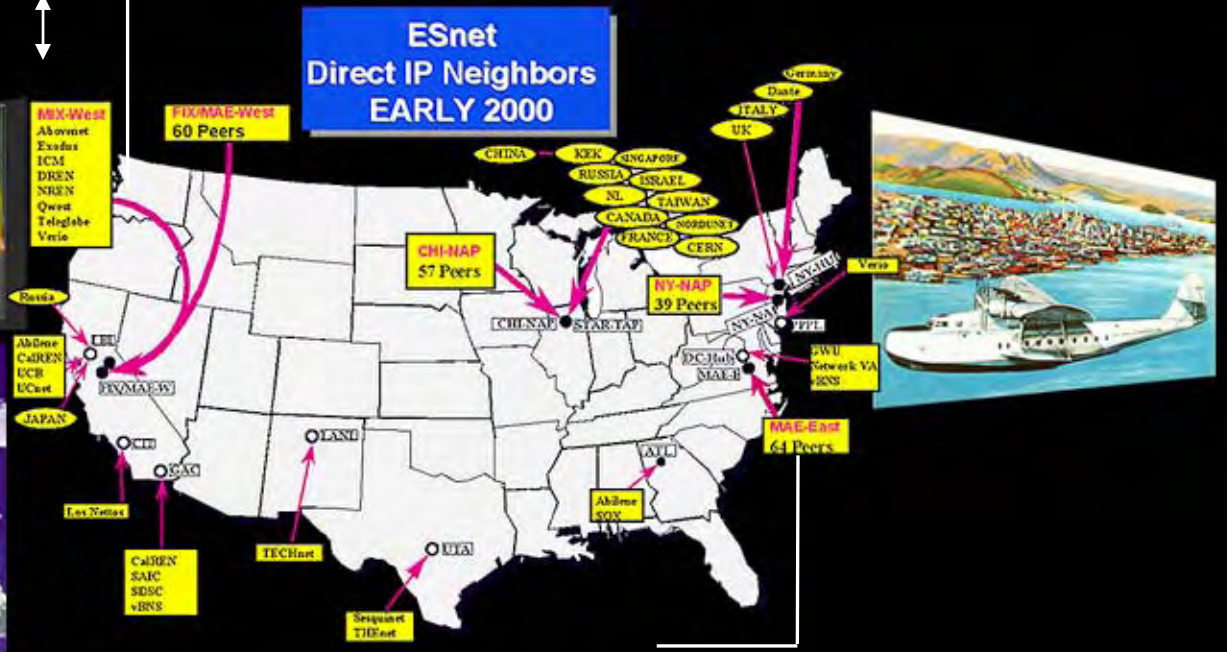
Grid services provide a uniform view of many diverse resources

Large-scale science and engineering is typically done through the interaction of

- People,
- Heterogeneous computing resources,
- Multiple information systems, and
- Instruments

All of which are geographically and organizationally dispersed.

The overall motivation for “Grids” is to enable the routine interactions of these resources to facilitate this type of large-scale science and engineering.



ESNet provides critical infrastructure

- **Advanced network infrastructure and specialized network services such as adaptive monitoring supporting high performance distributed applications, and Quality-of-Service and bandwidth reservation for building large-scale aggregated systems**
- **Collaboration services such as support for IP multicast based video teleconferencing**
- **Persistent support for directory services that provide naming and location of resources across the Grid and services that enable secure access to these resources**

Middleware and Network Research Awards

SciDAC-Integrating Science and Computing

Six Middleware and Network Research Projects that contribute to the development of the Collaboratory Software Environment - $3.4M

Middleware Technology to Support Science Portals	Indiana Univ. (Dennis Gannon)	$182k/Yr
A High Performance Data Grid Toolkit: Enabling Tech. For Wide Area Data Intensive Applications	Univ. of Wisconsin USC (Ian Foster, ANL)	$748k/Yr
Security and Policy for Group Collaboration	Univ. of Wisconsin USC (Steve Tuecke, ANL)	$750k/Yr
Optimizing Performance and Enhancing Functionality of Distributed Applications Using Logistical Networking	Univ. of Tennessee (Micah Beck)	$500k/Yr
Bandwidth Estimation: Measurement Methodologies and Applications	Wellesley College Univ. of Delaware (K. Claffy, UCSD)	$433k/Yr
INCITE: Edge-Based Traffic Processing and Service Inference for High Performance Networks	LANL SLAC (Richard Baraniuk, Rice Univ.)	$800k/Yr

Applied Mathematics Integrated Software Infrastructure Centers

SciDAC-Integrating Science and Computing

Three projects that will take up the challenge of providing scalable numerical libraries - $8.6M

Algorithmic and Software Framework for Applied Partial Differential Equations (APDE)	LLNL NYU U. of Washington U. of Calif. Davis U. of Wisconsin U. of North Carolina (Phil Colella, LBNL)	$2.7M/Yr
Terascale Optimal PDE Simulations (TOPS)	LLNL ANL LBNL Carnegie Mellon U. New York U. U. of Calif. Berkeley U. of Colorado U. of Tennessee (David Keyes, Old Dominion U.)	$3.3M/Yr
Terascale Simulation Tools & Technologies Center (TSTT)	ANL LLNL ORNL PNNL SNL RPI SUNY Stony Brook (Jim Glimm, BNL)	$2.6M/Yr

Computer Science Integrated Software Infrastructure Centers

SciDAC-Integrating Science and Computing

Four activities focused on a comprehensive, portable, and fully integrated suite of systems software and tools for effective utilization of terascale computers - $10.7M

Scalable Tools for Large Clusters; Resource Management; System Interfaces; System Management Tool Framework (SSS)	ANL LBNL Ames PNNL SNL LANL National Center for Supercomputing App (Al Geist, ORNL)	$2.2M/Yr
High-End Computer Systems Performance: Science & Engineering (PERC)	ANL LLNL ORNL U. of Illinois UCSD U. of Tennessee U. of Maryland (David Bailey, LBNL)	$2.4M/Yr
Center for Component Technology for Terascale Simulation Software (CCA)	ANL LANL LLNL ORNL PNNL U. of Utah Indiana U. (Rob Armstrong, SNL)	$3.1M/Yr
Scientific Data Management Enabling Technology Center (SDM)	ANL LLNL ORNL Georgia Tech. UCSD Northwestern U. North Carolina State (Ari Shoshani, LBNL)	$3M/Yr

Scalable Systems Software
for TeraScale Computers

www.scidac.org/ScalableSystems

Problem

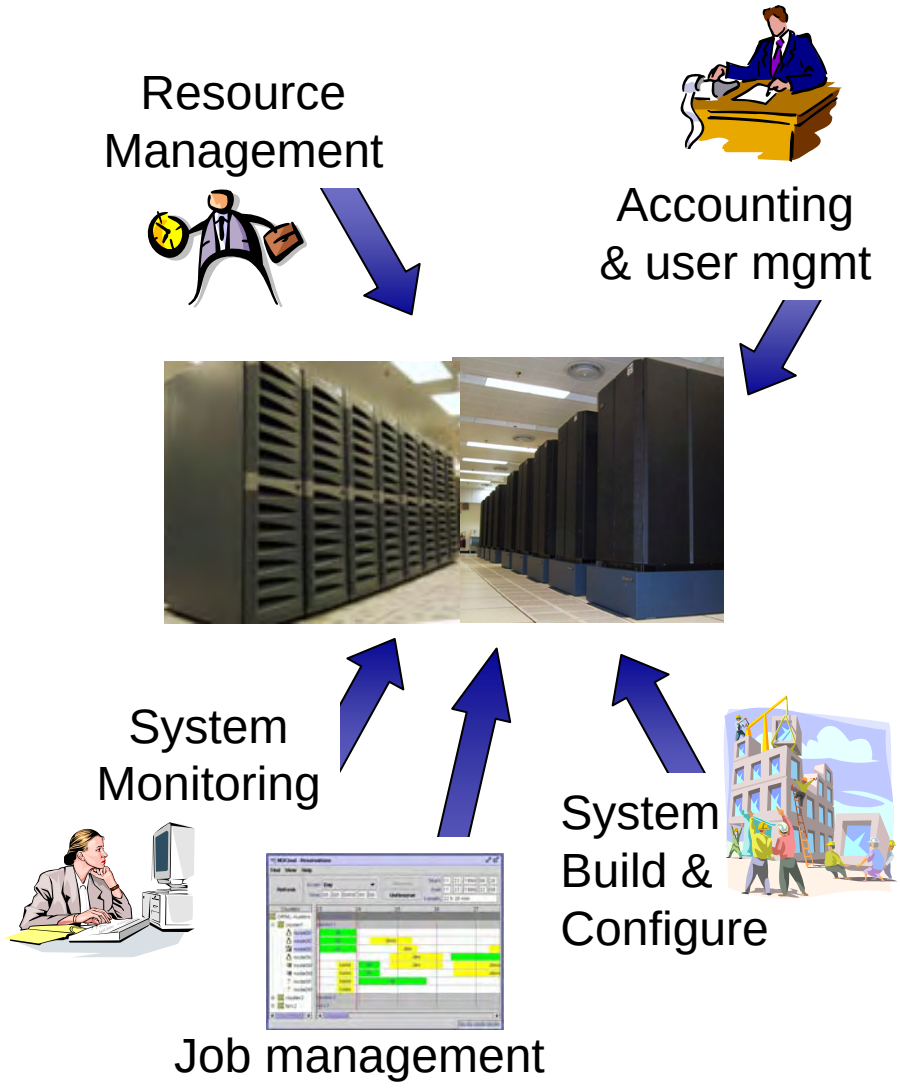
- Computer centers use incompatible, ad hoc set of systems tools
- Present tools are not designed to scale to multi-Teraflop systems

Solution

- Collectively (with industry) define standard interfaces between systems components for interoperability
- Create scalable, standardized management tools for efficiently running our large computing centers

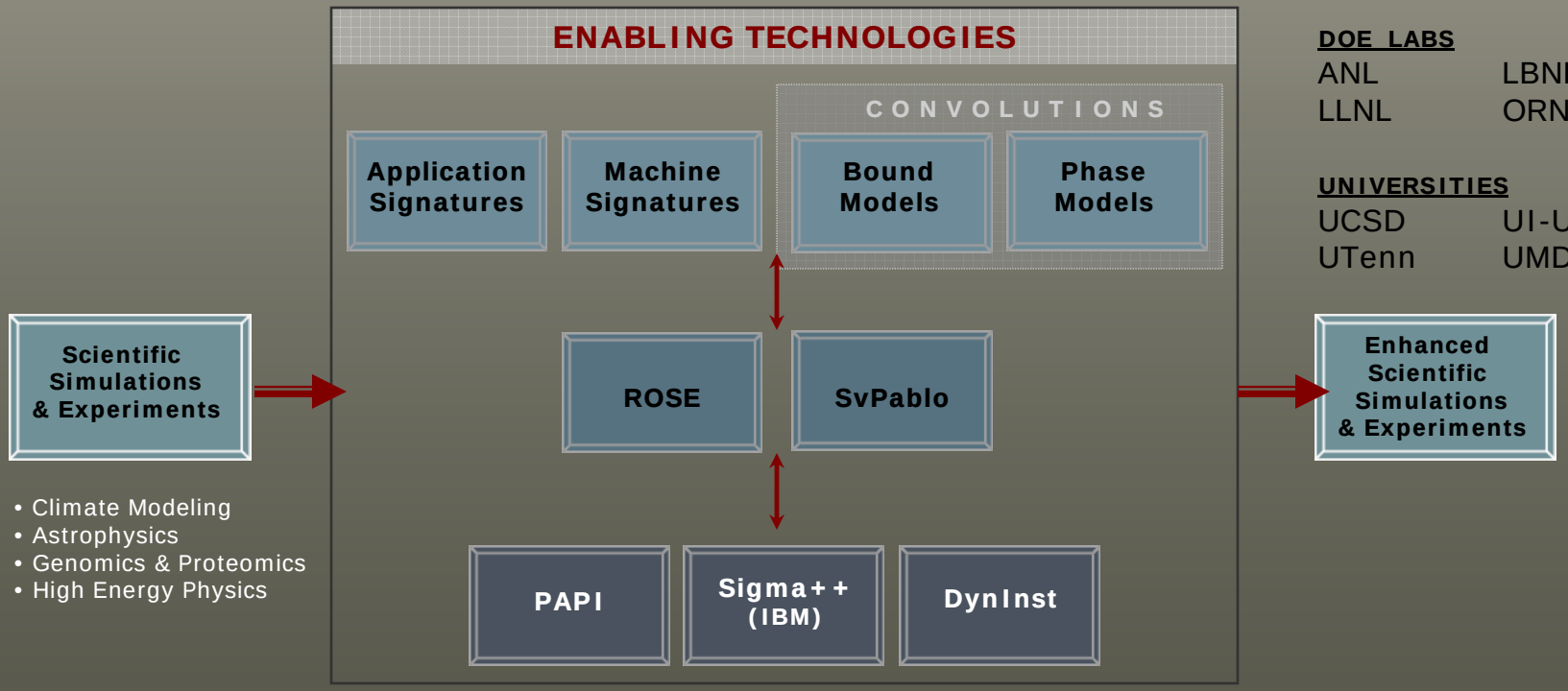
Impact

- Revolutionize the way system software is designed and used.



PERC PERFORMANCE EVALUATION RESEARCH CENTER

Developing a *science* for understanding performance of scientific applications on high-end computer systems, and *engineering* strategies for improving performance on these systems.



DOE LABS

ANL LBNL
LLNL ORNL

UNIVERSITIES

UCSD UI-UC
UTenn UMD

GOALS

Optimize and Simplify:

- Profiling of real applications
- Measurement of machine capabilities (emphasis on memory hierarchy)
- Performance prediction
- Performance monitoring
- Informed tuning

Understand the key factors in applications that affect performance.
Understand the key factors in computer systems that affect performance.
Develop models that accurately predict performance of applications on systems.
Develop an enabling infrastructure of tools for performance monitoring, modeling and optimization.
Validate these ideas and infrastructure via close collaboration with DOE SC and other application owners.
Transfer the technology to end-users.

Component Technology for Terascale Simulation Software:
Bringing Components to High Performance Computing

http://www.cca-forum.org/ccttss

CCA

Common Component Architecture

Participants:

ANL

Indiana Univ.

LANL

LLNL

ORNL

PNNL

SNL

Univ. of Utah

Partners:

Climate Modelling

Quantum Chemistry

Combustion Modelling

Currently DOE Apps Are:

- One-off, stove-pipe, few participants

But Also:

- Scalable, and low latency
- Large & rich legacy investment

Challenges

- Practical parallel HPC component model
- Integrate legacy software investment
- Connection to Grid components
- Multi-language

Goals

- Enable plug-and-play parallel simulations
- Establish component "marketplace" with applications partners
- Extend commodity component technology for HPC

Today:

Single-purpose, monolithic, tightly-coupled parallel codes

HPC Component Framework

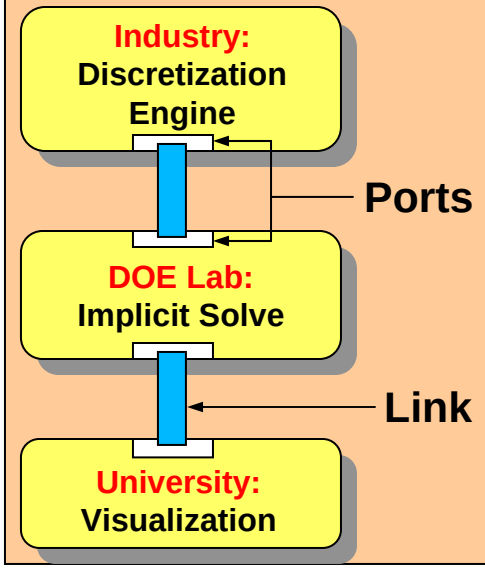
Scientific Components

CCA

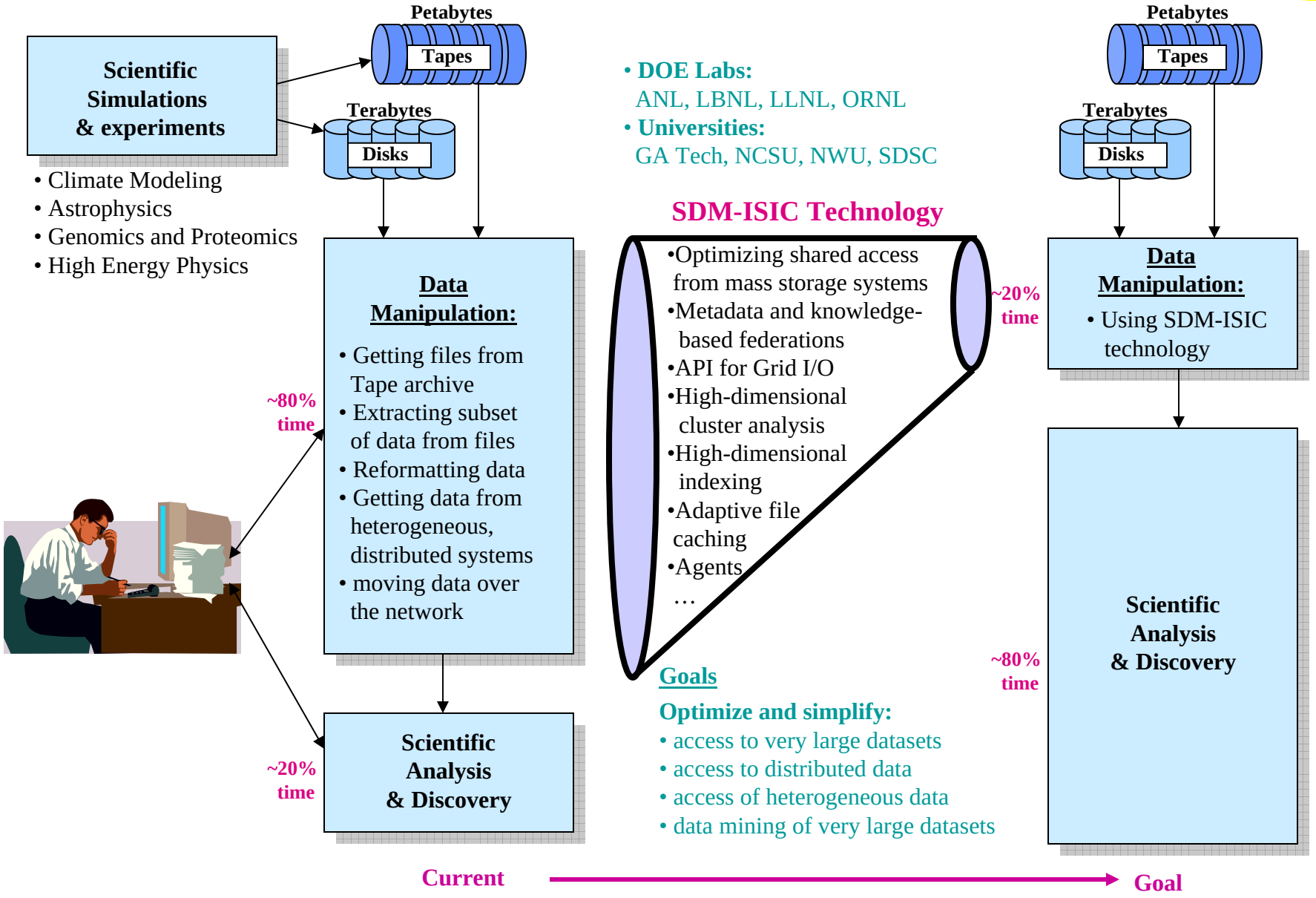
"MxN" Parallel Data Redistribution

Applications Integration

Component-Based Scientific Application



Scientific Data Management ISIC



Summary of Interactions

SciDAC-Integrating Science and Computing

			ISIC Ties						
Office	**Project Title**	**SA $**	CCA	SDM	PERC	SSS	TSTT	TOPS	APDE
FES	Magnetic Reconnection: Applications to Sawtooth Oscillations, Error Field Induced Islands and the Dynamo Effect	60							
FES	Numerical Computation of Wave-Plasma Interactions in Multi-dimensional Systems	225						Yes	
FES	Center for Extended Magnetohydrodynamic Modeling	80					Yes	Yes	
FES	The Plasma Microturbulence Project	35						Yes	
HENP	Advanced Computing for 21st Century Accelerator Science and Technology	655			Yes		Yes	Yes	Yes
HENP	National Computational Infrastructure for Lattice Gauge Theory	134							
HENP	Shedding New Light on Exploding Stars: Terascale Simulations of Neutrino-Driven SuperNovae and their NucleoSynthesis	416	Yes		Yes		Yes		
HENP	SciDAC Center for Supernova Research	150							
BER	Collaborative Design and Development of the Community Climate System Model for Terascale Computers				Yes		Yes		
BES	A Computational Facility for Reacting Flow Science		Yes	Yes			Yes	Yes	
BES	Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry	138			Yes				
BES	Advanced Methods for Electronic Structure	250			Yes				
BES	Advancing Multi-Referance Methods in Electronic Structure Theory					Yes			
BES	Accurate Properties for Open-Shell States of Large Molecules		Yes						
BES	Advanced Software for the Calculation of Thermochemistry, Kinetics and Dynamics		Yes						
ASCR	DOE Science Grid: Enabling and Deploying the SciDAC Collaboratory Software Environment			Yes		Yes			
ASCR	A National Collaboratory to Advance the Science of High-Temperature Plasma Physics for Magnetic Fusion	35							
ASCR	Particle Physics Data Grid Collaborative Pilot			Yes					
ASCR	Earth System Grid II: Turning Climate Datasets into Community Resources			Yes					
ASCR	A High-Performance Data Grid Toolkit: Enabling Technology for Wide Area Data-Intensive Applications			Yes					
ASCR	Scalable Systems Software Center (SSS)		Yes			Yes			
ASCR	High-End Computer Systems Performance: Science and Engineering (PERC)				Yes		Yes	Yes	Yes
ASCR	Center for Component Technology for Terascale Simulation Software (CCA)		Yes			Yes	Yes	Yes	
ASCR	Scientific Data Management Center (SDM)			Yes		Yes			
ASCR	Terascale Optimal PDE Simulations (TOPS)		Yes		Yes		Yes	Yes	Yes
ASCR	Terascale Simulation Tools & Technologies Center (TSTT)		Yes		Yes		Yes	Yes	
ASCR	Algorithmic and Software Framework for Applied Partial Differential Equations (APDE)				Yes			Yes	Yes