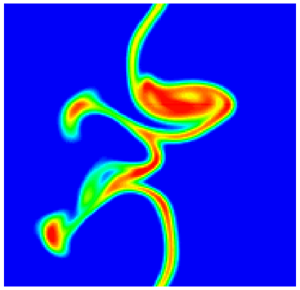
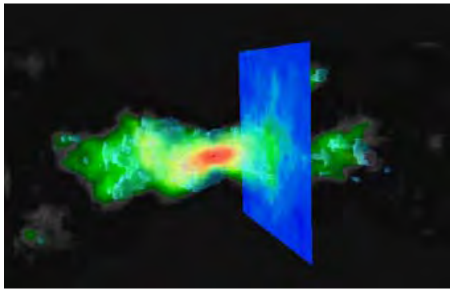
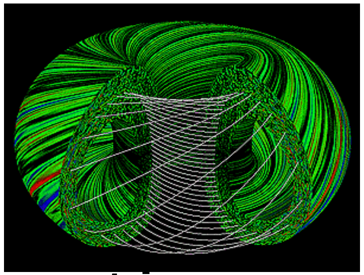
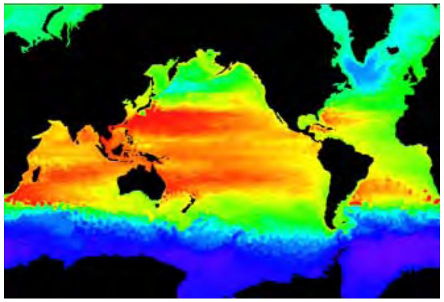






# A Short History of Mathematics, Computing and Information Sciences Research at DOE

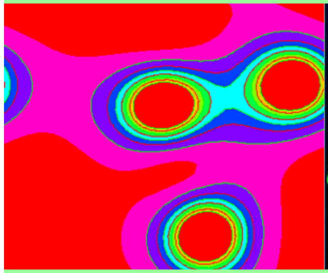


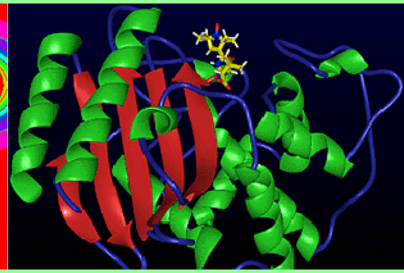

*Dr. Daniel A. Hitchcock*

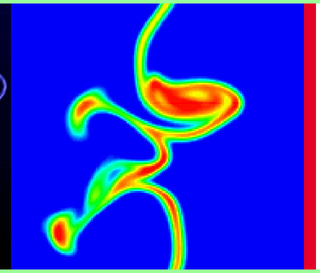

*November 1, 2000*

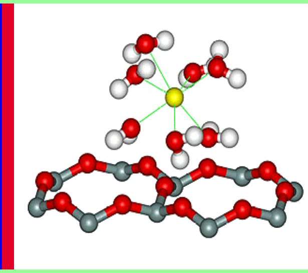


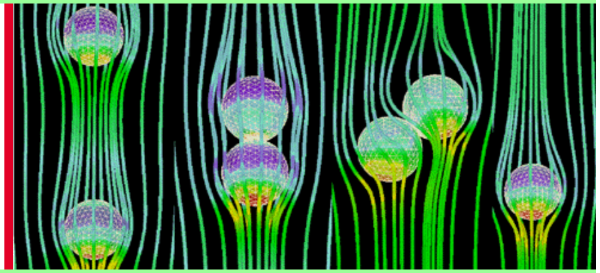
# Advanced Computing Is Critical for Scientific Discovery

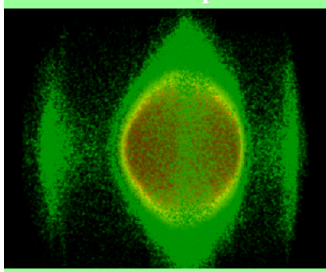

Vortices in a superfluid

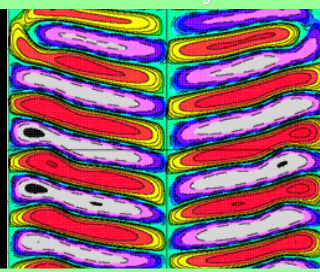

Protein dynamics


Turbulent methane flame

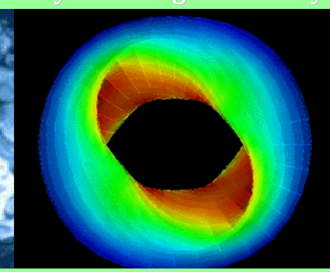

Clay-mineral geochemistry

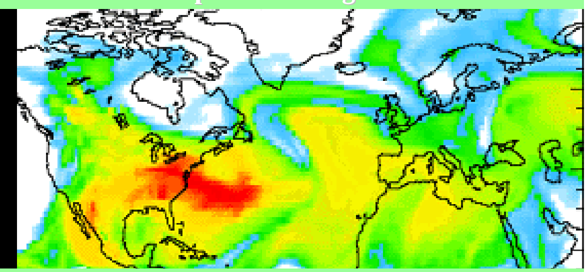

Two spheres mixing in a stream

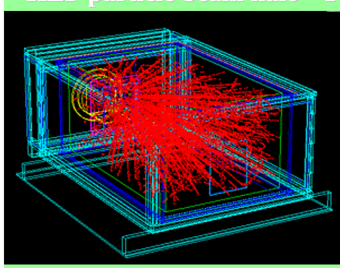

HEP particle beam halo

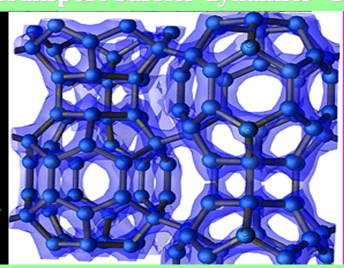

Transport barrier dynamics

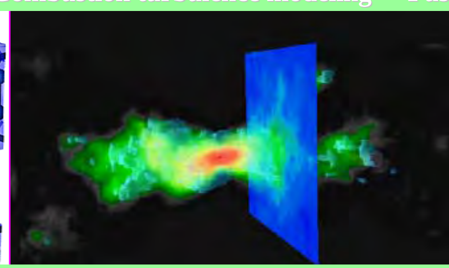

Combustion turbulence modeling

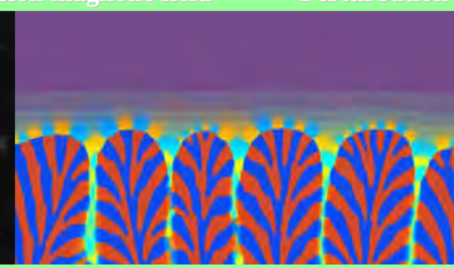

Fusion magnetic field

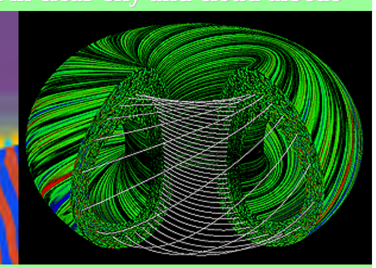

Perturbation in clear-sky and cloud albedo

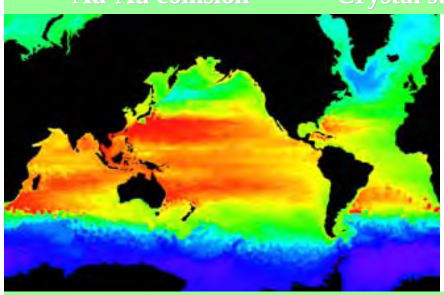

Au-Au collision

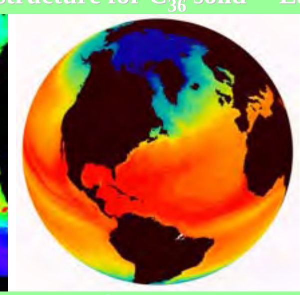

Crystal structure for $C_{36}$ solid

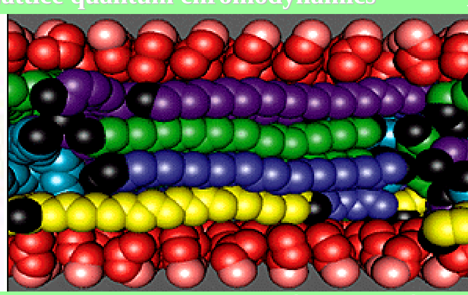

Lattice quantum chromodynamics

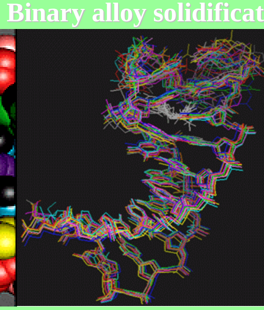

Binary alloy solidification

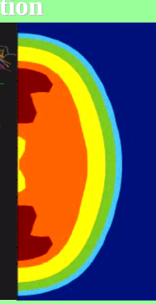

Perturbed plasma density

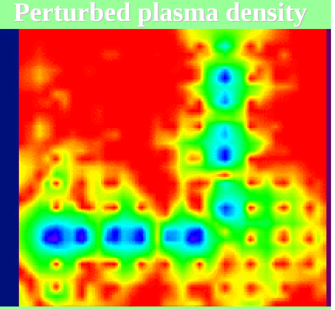

DOE Parallel Climate Model


Sea surface temperature

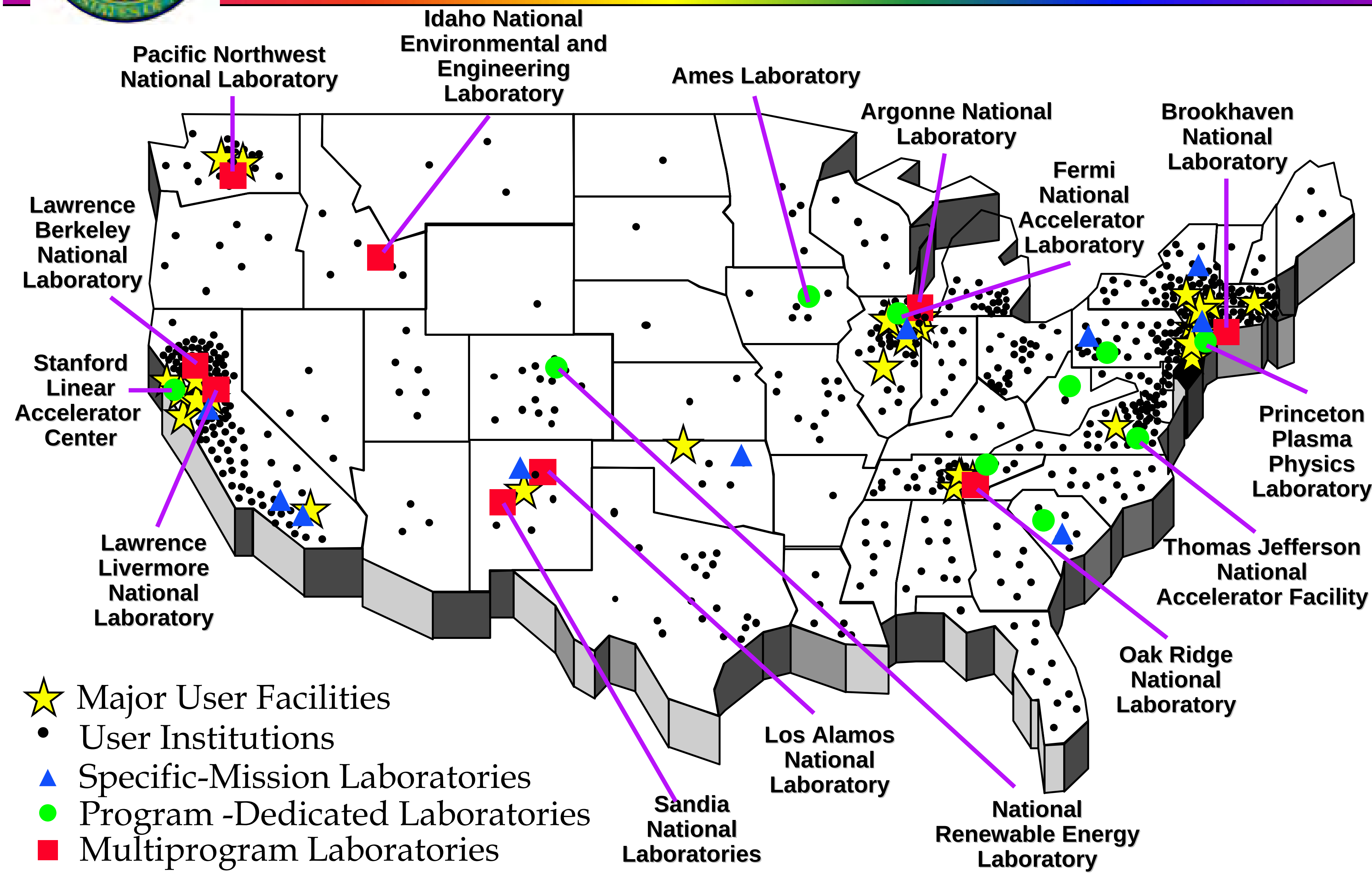

Molecular simulation of complex fluids


Structural biology


Nuclear theory


Waveguide optics

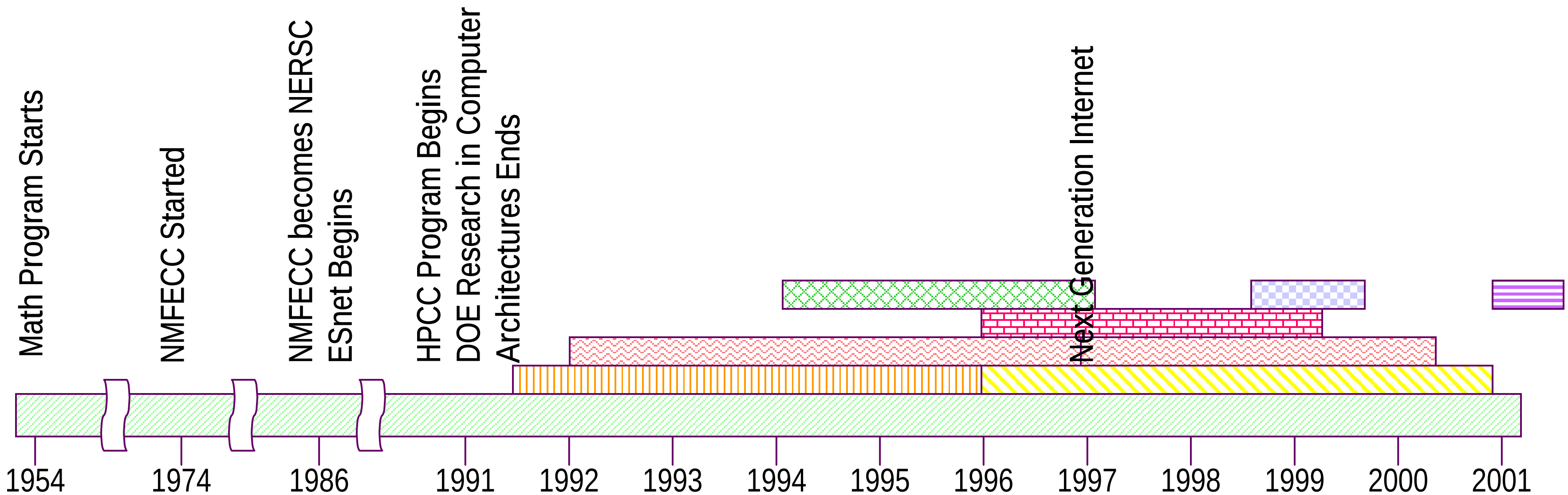
# Collaboratories and Networks are Critical for DOE



# A Short History of Mathematics and Computing Research at DOE

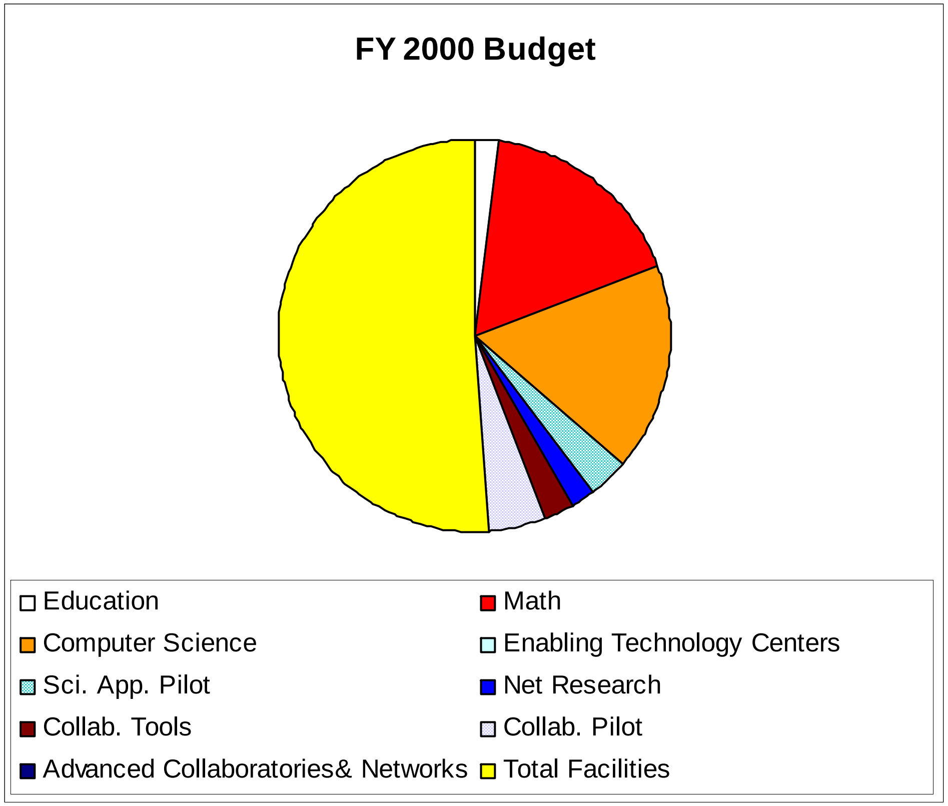
*"Von Neumann to the Present"*

- High Performance Computing Research Centers
- Advanced Computing Research Facilities
- "Grand Challenges"
- DOE 2000
- Electricity Supply and Demand Management
- Next Generation Internet
- SciDAC

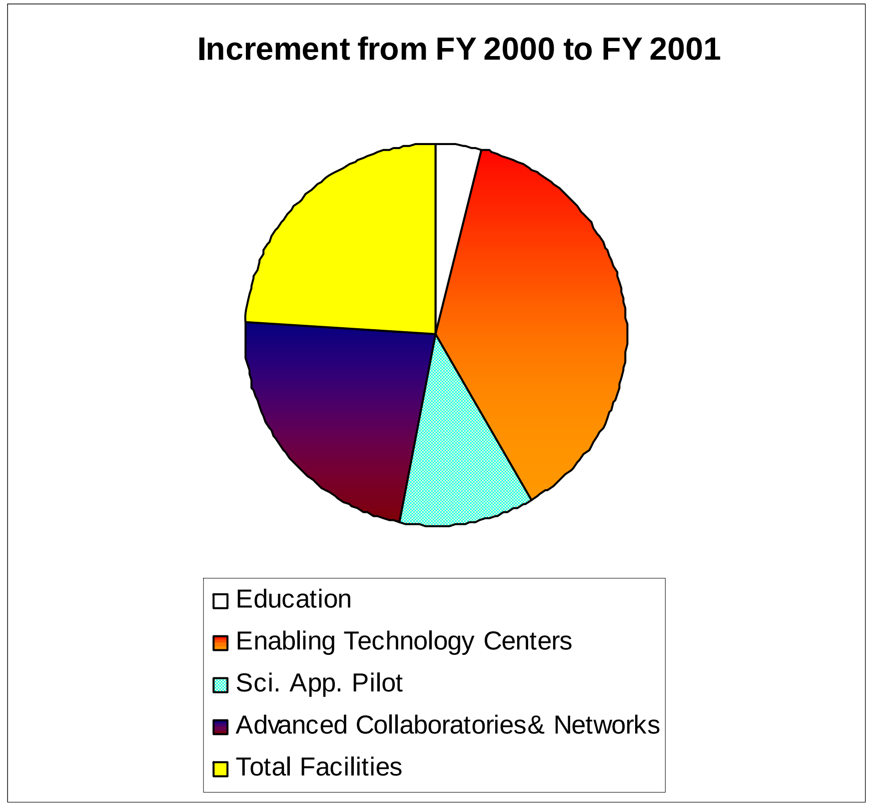


# MICS Budget Changes from FY 2000 to FY 2001

*FY 2000 ~ $116M*



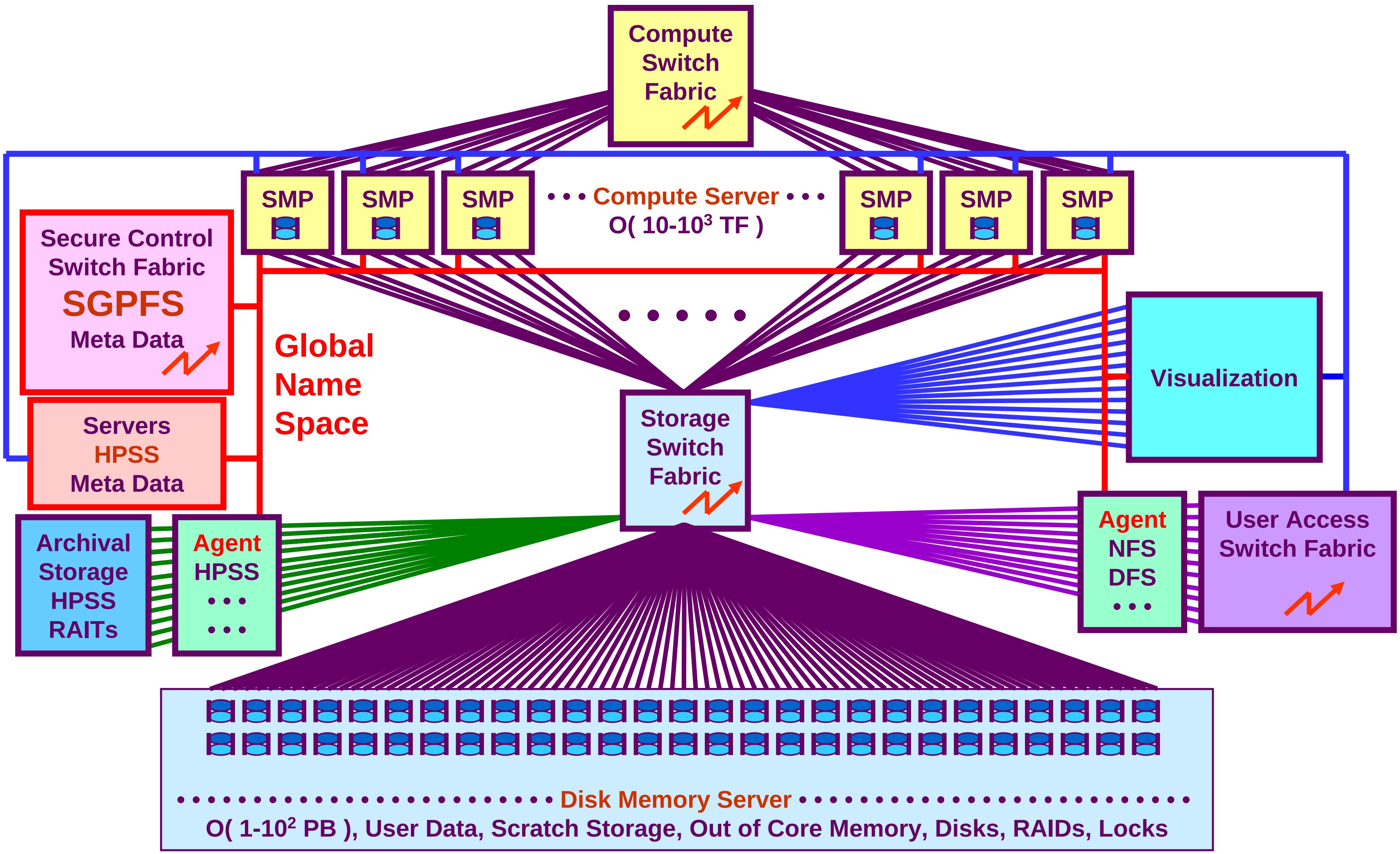

*Increment ~ $30M*



# The Challenges

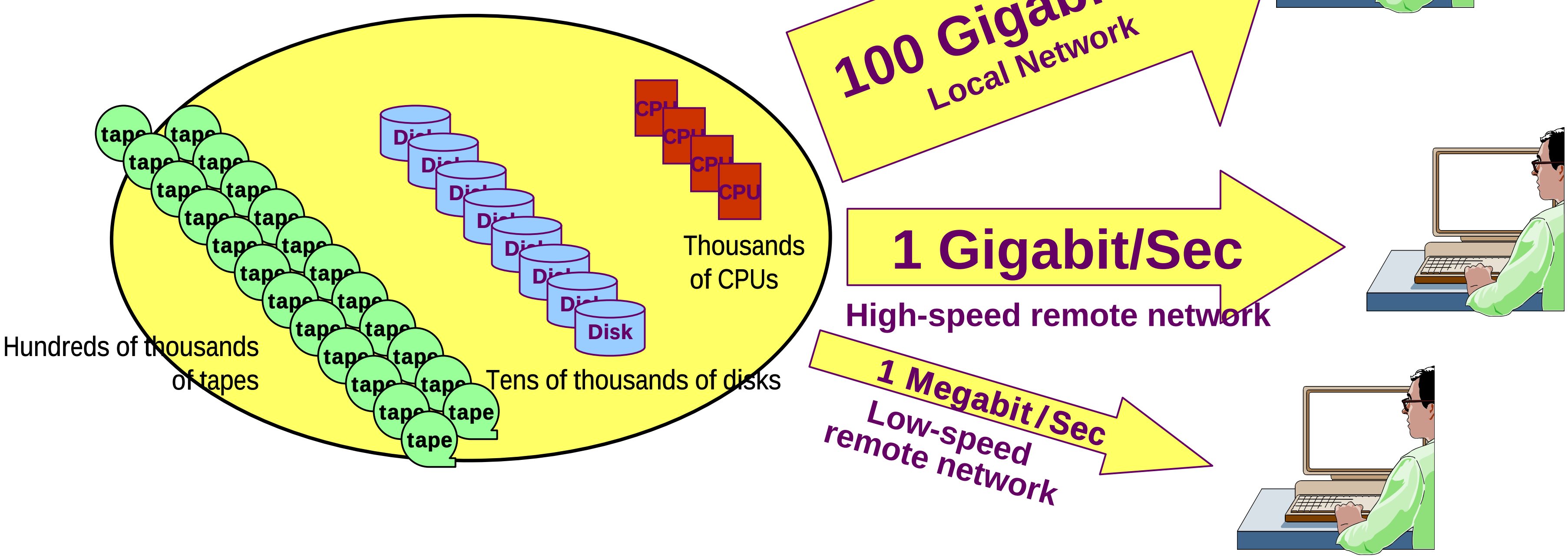
- Terascale Computers
- Tera -- PetaScale Data
- Applied Math
- Software
- Collaboratories and Networks

# Terascale Computer Challenge



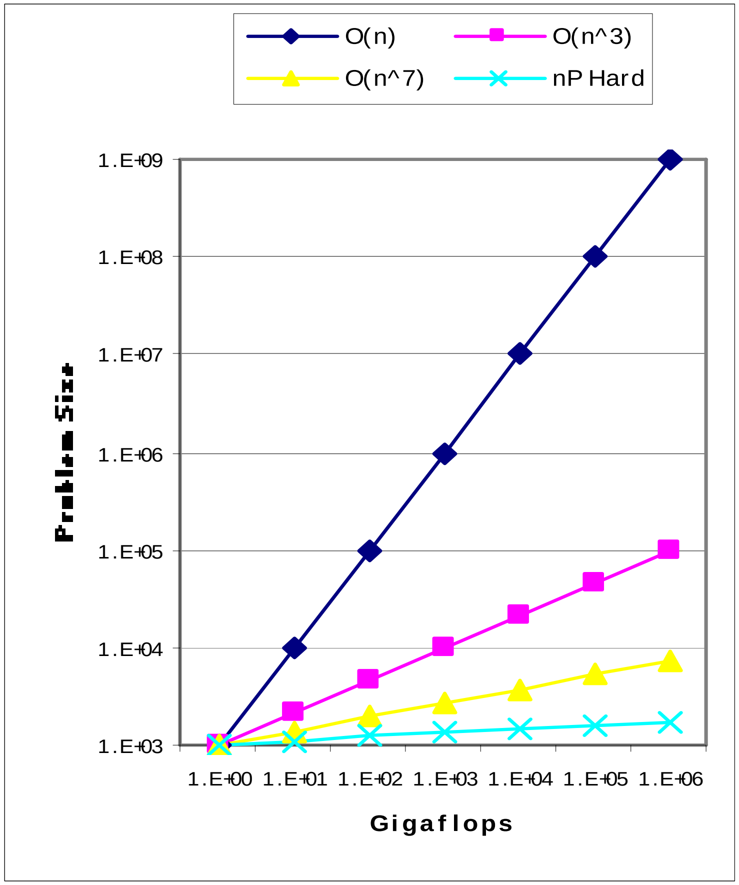
# Tera -- PetaScale Data Challenge

- High performance computers and new experimental facilities will produce millions of gigabytes of data.
- Enabling scientists to interact with this volume of data and find and analyze critical features is a formidable challenge.
- Remote access time is a serious concern.
- Disks and Tapes getting bigger but not faster
- Increases in parallelism required to integrate system

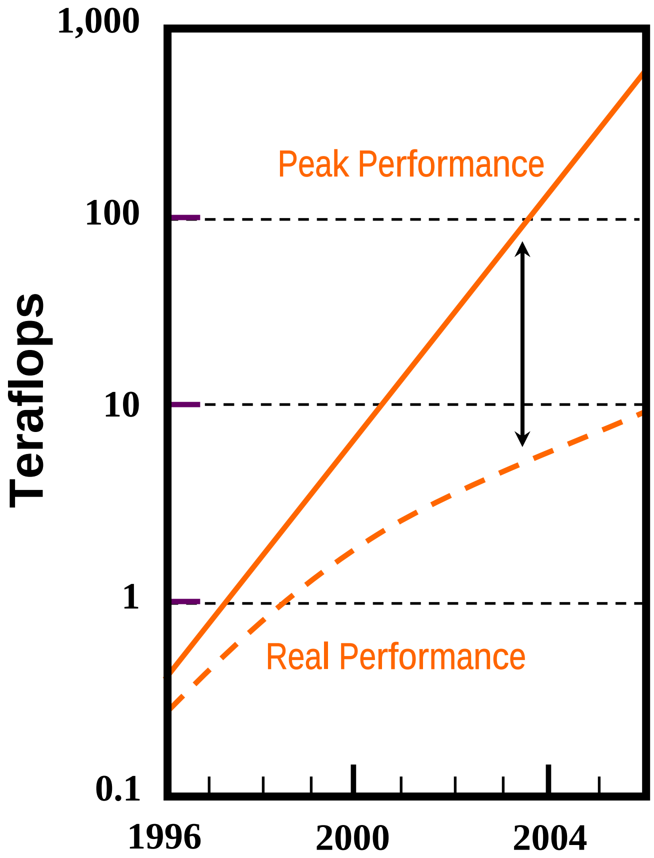


# Applied Math Challenges

Algorithm Scaling with Problem Size Determines the Size Problem that can be Solved!




Algorithms determine what fraction of peak performance is delivered to science



# Software Challenge

***The time it takes to move an application to a new generation of computers is time lost to scientific discovery.***

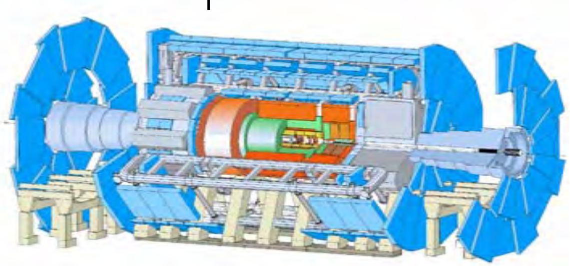
- Scientific modeling and simulation codes endure much longer than the life of a generation of computers (~3 years)
  - The "Gaussian" computational chemistry code for which John Pople was awarded the 1998 Nobel Prize has been in existence (and evolving) since 1970.
- DOE has pioneered many of the advanced software technologies required to accomplish this goal while achieving high performance
- Significant research, as well as education and software support, are required to achieve the promise of these initial efforts.

# National Collaboratory Challenges

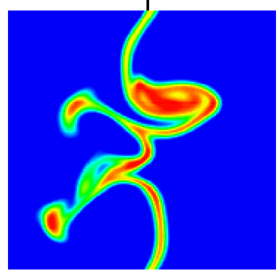
Collaboratories link geographically distributed researchers, data, and tools via networks to enable remote access to facilities, access to data sets, shared environments, and ease of collaboration

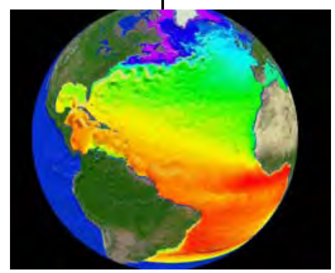
## High-Speed Nationwide Networks

Remote Access to Scientific Instruments



Data from Petabyte/year Experimental Facilities





Terascale Simulations

Shared Virtual Environments


Scientists' Desktops

# MICS is an *INTEGRATED* Program Research --> Users

*Disciplinary Science and Engineering*

*External to SC* | *ASCR* | *BES,BER,FES,HEP,NP*

## Underlying Technologies → Fundamental Research → R&D for Applications → Testbeds → Scientific Computing

**Underlying Technologies**

- Hardware
- Software
- Networking

**Fundamental Research / R&D for Applications / Testbeds**

- Applied Mathematics
- Computer Science
- Advanced Computing Software Tools

(FY 2000 $46.1M --------> FY 2001 $53.8M)

- Scientific Application Pilots
- Enabling Technology Centers

*Groups of mathematicians, computer scientists, application scientists, and software engineers* (FY 2001 $19.2M)

- Networking
- Collaboratory Tools

(FY 2000 $14M --------> FY 2001 $24.1M)

- Collaboratory Pilots

**Scientific Computing**

- Applications, e.g.
  - Materials Sciences
  - Chemical Sciences
  - Combustion Modeling
  - Accelerator Science
  - High Energy Physics
  - Nuclear Physics
  - Fusion Energy
  - Global Climate
  - …
  - …

( FY 2001 +$20M)

- Access to Facilities
- Link Researchers

**Facilities** (FY 2000 $56.0M ---> FY 2001 $68.3M)

- National Energy Research Scientific Computing Center (NERSC)
- Advanced Computing Research Facilities
- Energy Sciences Network (ESnet)

# MICS Tries to Adopt an Architectural View of the Problem

**DOE Missions**: Defense, S&T Leadership, Climate, Cleanup

**Scientific Disciplines**: Physics, Chemistry, Biology, Materials

**SW Development**: ACTS Toolkit

**Collaboratory Tools**: Electronic Notebook

**Data Mgmt. & Visualization**: CAVE, EigenVR

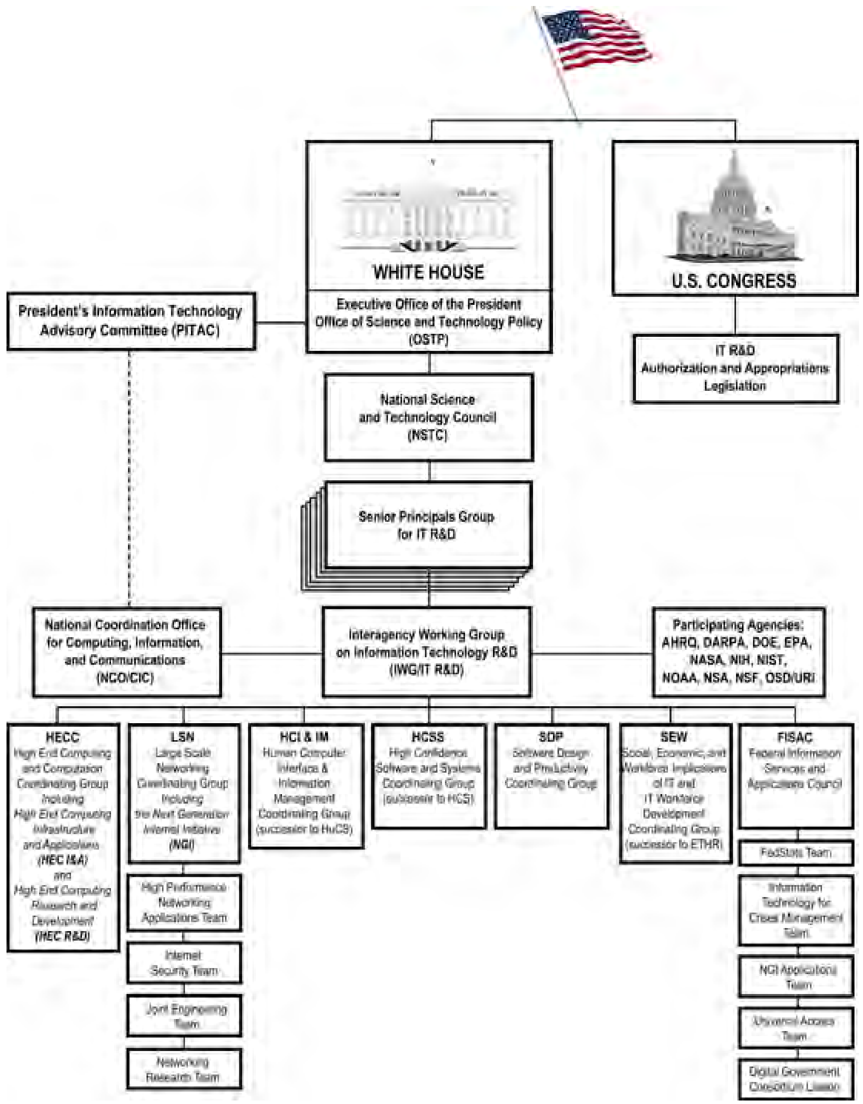
**Math & Comp Sci.**: Algorithms, Portals, Globus

**Libraries & Tools**: Debuggers, Graphics, PVM, MPI

**Systems Software**: Adv. Nets., I/O - HPSS, POOMA

**Facilities**: Computers, Experiments, Networks, Databases, Storage

# MICS is an Intgral Part of Federal IT Research Enterprise



# Who Manages What in MICS

- Division Director:  C.E. Oliver (Acting)
  - Applied Mathematics:  D. Hitchcock (Acting)
  - Computer Science:
    - Clusters, System Software, Tools: F. Johnson (on Detail from NIST)
    - Data Management, Viz & I/O: D. Hitchcock
    - Advanced Computing Software Tools: M.A.  Scott
  - Network Research: T. N'Dousse
  - Collaboratory Tools & Collaboratory Pilots: M.A. Scott
  - Scientific Application Pilots: T. Kitchens & Staff
  - Facilities:
    - NERSC:  T. Kitchens
    - ESnet:  G. Seweryniak
    - ACRF's:  W. Polansky  and T. Kitchens

# Computational Science Education
# FY 2000: $2M

## *Objective:*

Develop future generations of leaders in applied mathematics and computational science

## *Accomplishments:*

## *Ongoing Projects*

*Computational Sciences Graduate Fellowship Program:*

## *Future Plans*

Doubling of CSGF

# Applied Mathematics
# FY 2000: $19M

## *Objectives:*

Support mathematical and computational research that facilitates the use of the latest high-performance computer systems in advancing our understanding of science and technology.

## *Accomplishments:*

Libraries

AMR

NP hardness of 3-d Ising Model

Differential-Algebraic Equations

Theory of Chaos

## *Ongoing Projects*

### *Applied Mathematics Research:*

Linear Algebra
CFD
PDE's
Optimization
Grid Generation

### *Coupling Applied Math to Applications:*

Materials Science
Biology
Combustion
High Energy Physics

## *Future Plans*

Math Libraries for Terascale computers

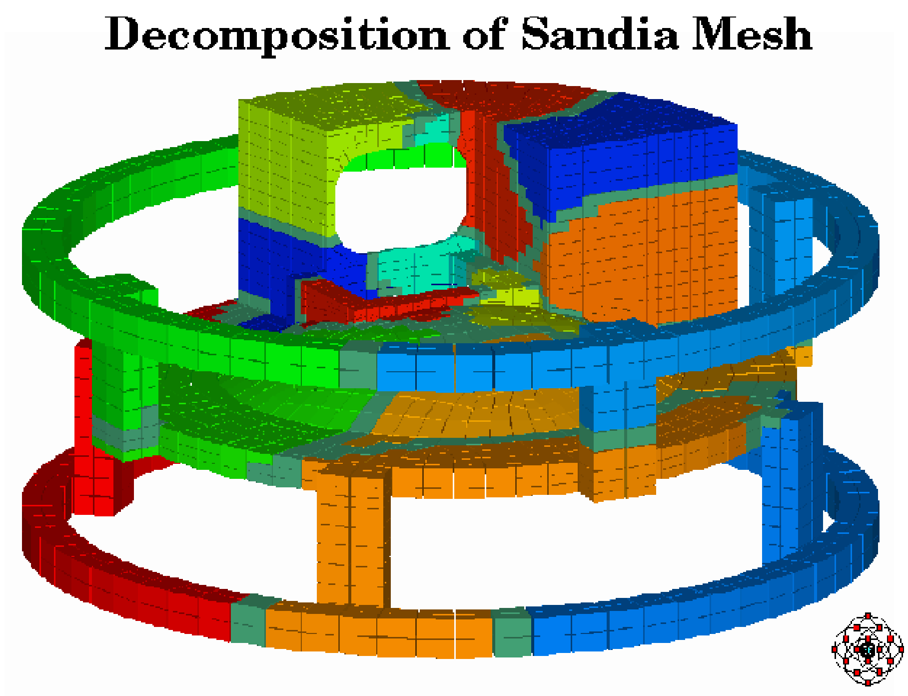
Enabling Technology Centers?

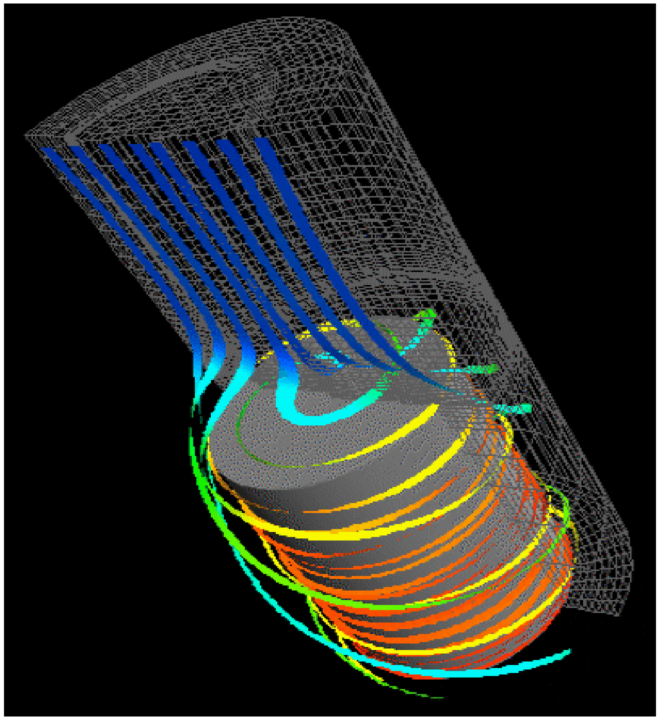
Predictability

Feature Description

Get Permanent Program Manager in Place

# A Few Examples



# Computer Science Research & Tools FY 2000: $19M

## Objectives:

Enable Scientists to rapidly construct software, execute it with high performance on terascale computers, and manage the resulting data

## Accomplishments:

PVM, MPI

Storage Access Control System

Dyninst/Paradyne

ACTS Toolkit

## Ongoing Projects

Systems Software
Data Management, Visualization & I/O
Advanced Computing Software Tools

## Future Plans

Enabling Technology Centers

Recompete ACTs Toolkit

Operating Systems

# System Software Environment

## *Goals and Objectives*

A common system software and tool technology base for terascale systems which:

- Delivers high sustained application performance, ease of use, and manageability
- Enables and supports a unified environment forscientific computation from desktop to teraop systems

## *Accomplishments*

- PVM
- MPI, MPI-2
- MPICH
- Netsolve (99 IR100 award)
- Paradyn, DynInst
- Terascale systems software roadmap

## *Ongoing Projects*

### *System Software Technology*

- Scalable cluster management tools
- Resource management
- Harness, Cumulvs, Netsolve

### *Parallel Programming/Performance*

- MPICH -- performance, thread safety
- Unified Parallel C
- Heterogeneous distributed computation
- Performance instrumentation

## *Future Plans*

- Scalable systems management
  - resource management, scheduling
  - common management infrastructure
- Performance measurement, benchmarks, modeling and prediction
- Microkernels for terascale systems
- High performance messaging and remote memory access
- Open source emphsis

# ARMCI

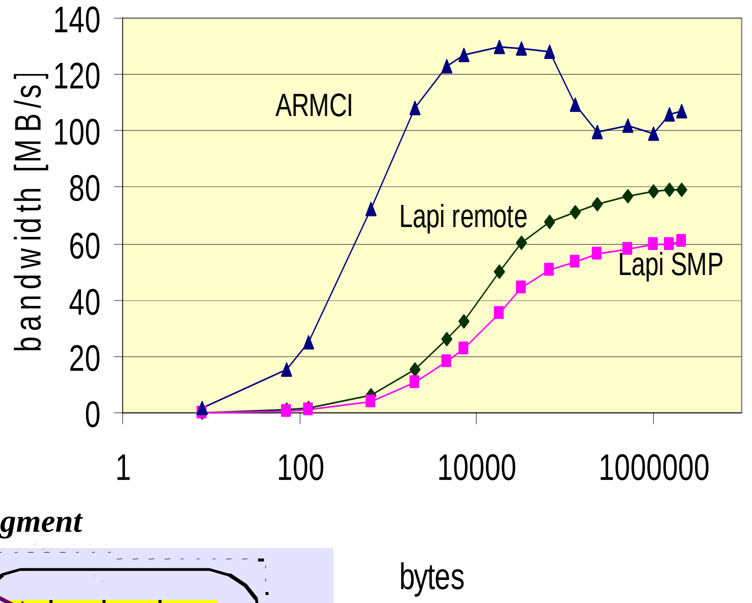
## First portable 1-sided communication library

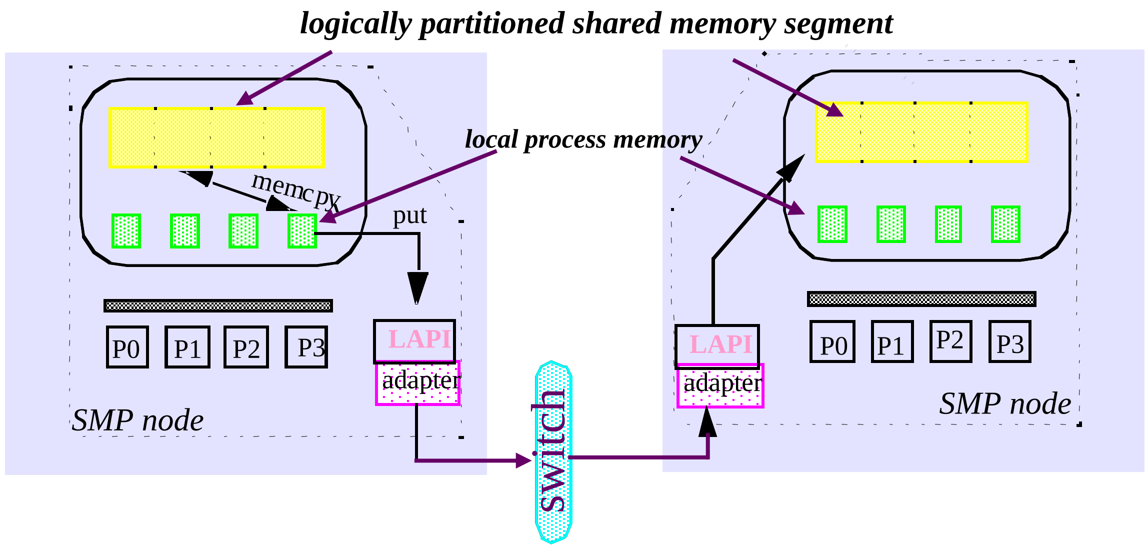
- Core communication capability of Global Arrays (GA) were generalized, extended, and made standalone
- Approach
  - simple progress rules
    - less restrictive than MPI-2 (includes 1-sided communication)
  - low-level
  - high-performance
    - optimized for noncontiguous data transfers (array sections, scatter/gather)
  - implemented using whatever mechanisms work best on given platform:
    - active messages, threads, sockets, shared memory, remote memory copy
- Used by GA as its run-time system and contributed to other projects
  - Adlib (U. Syracuse)
  - Padre/Overture (LLNL)
  - U. Florida

# Intelligent Protocols in ARMCI

On IBM SP with SMP nodes ARMCI exploits

- cluster locality information
- Active Messages
- remote memory copy
- shared memory within SMP node
- threads



# Data Management, Visualization and I/O Technologies

## *Objectives:*

Develop tools to enable scientists to extract knowledge from petabytes of scientific data

Enable high speed I/O from terascale computers and storage systems

## *Accomplishments:*

Storage Access Coordination System (STACS)

CAVELib

Billion Cell Rendering

MUSE

MPI-IO, ROMIO

## *Ongoing Projects*

### *Data Mgt:*

Indexing & Query estimation
Distributed Data Mining
Advanced database concepts
HENP Data Grand Challenge, PPDG, ESG

### *Visualization:*

VR& Haptics
Rendering very large datasets
Feature Extraction

### *I/O:*

Scalable I/O Consortium
HPSS
Network Attached Disk Caches

## *Future Plans*

Petabyte Data Challenge

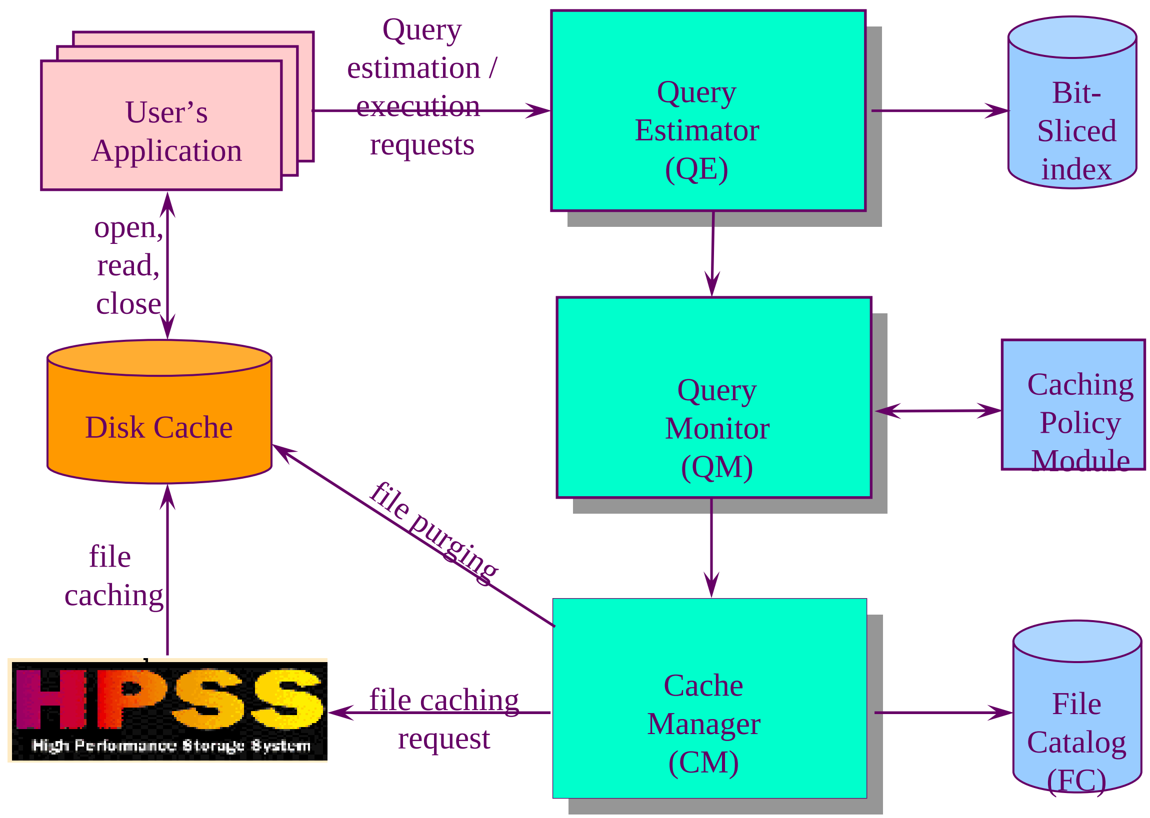
Multi-Dimensional Clustering

Feature Extraction

Vector and Tensor Fields

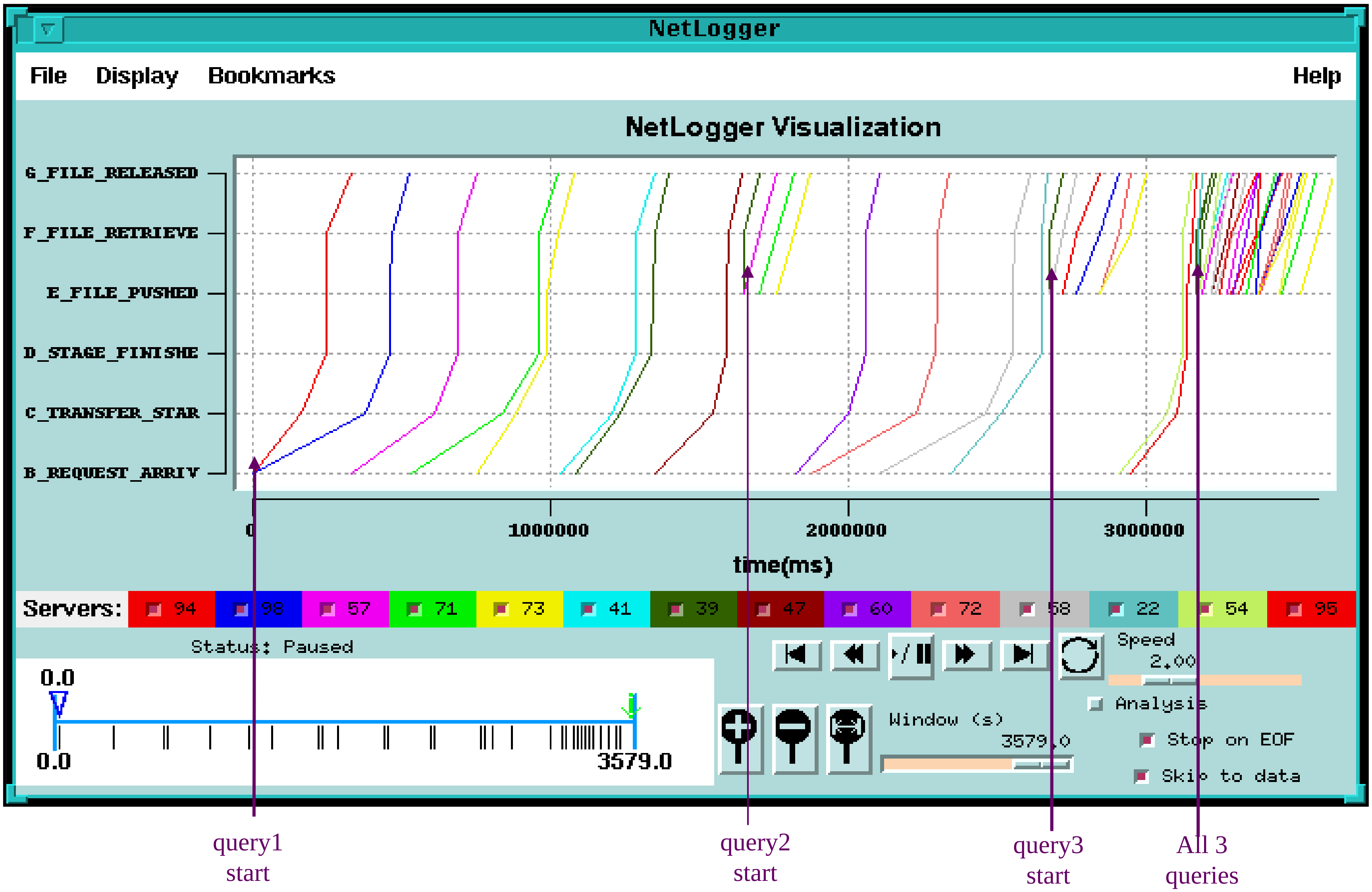
Hierarchical Methods

# Challenge of Petabytes of Data
## Access Coordination System (STACS)



# Challenge of Petabytes of Data

## STACS Parallel Performance

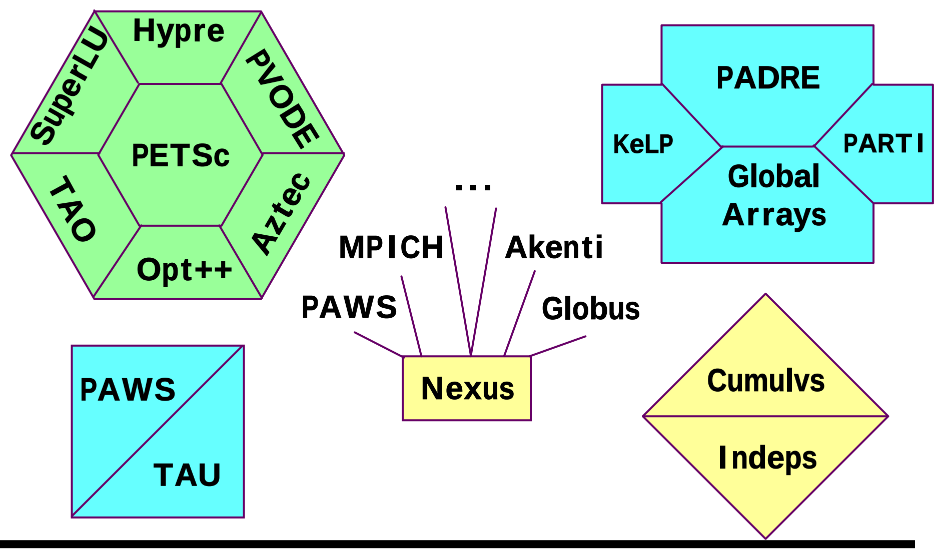


# ACTS Toolkit Program: Software Interoperability for HPC

## Objectives:

Develop an *integrated* set of software tools, algorithms, and environments that accelerate the adoption and use of advanced computing for mission-critical problems.

## Accomplishments:




## Ongoing Projects

- Numerics
- Code Execution
- Code Development
- Test and Consult
- Applications Support Tools

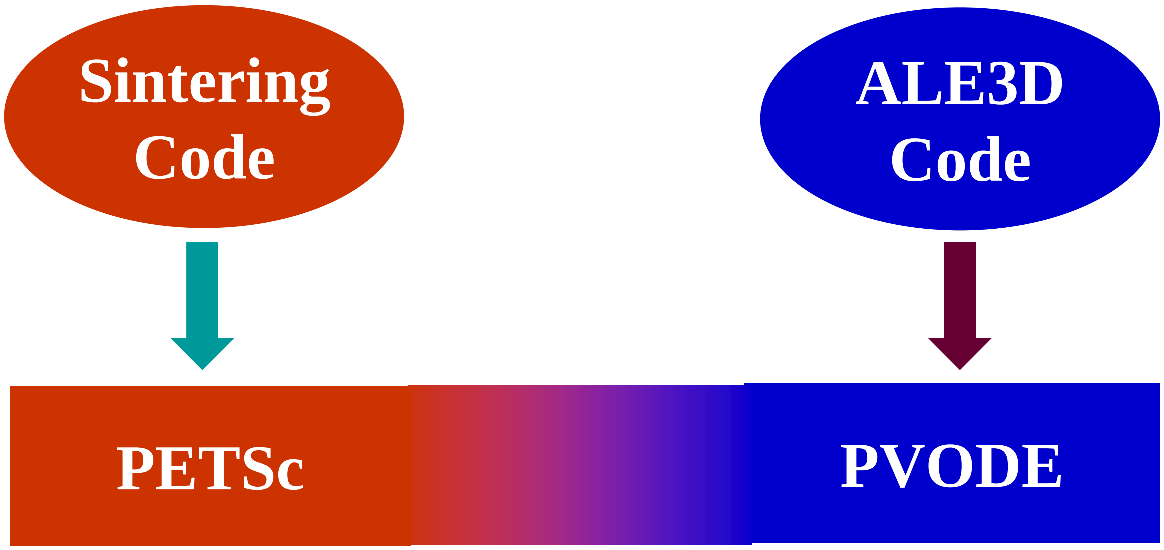
## Future Plans

- Develop a support technology for simplifying the process of making tools interoperable
- Recompete funds to expand the types of tools that are made interoperable

# ACTS Toolkit Program: Success Story

Wen Zhang, Oakland University
Joachim Schneibel, ORNL

Mark Adams (Berkeley)




Sintering - simulating the dynamics of micro-structural interactions, requiring the solution of a large set of coupled ODEs

Previously used LSODE, limited to 100s of degrees of freedom, now can handle 10,000s

ALE3D test problems run with PETSc based parallel multi-grid solver

- Run on NERSC 512 processor T3E and LLNL ASCI Blue Pacific
- Simulation with 16 million+ degrees of freedom

# Scientific Application Partnerships FY 2000: $4M

## *Objectives:*

Bring together discipline scientists, computer scientists and mathematicians to apply the results of MICS funded research on scientific problems critical to DOE.

Produce new Discipline Science and new Computational Science

## *Accomplishments:*

Gordon Bell Prize: Magnetic Materials

Billion Particle Accelerator Simulation

.1$^{o}$ Simulation of Global Ocean

## *Ongoing Projects*

All Projects Ended in FY 2000

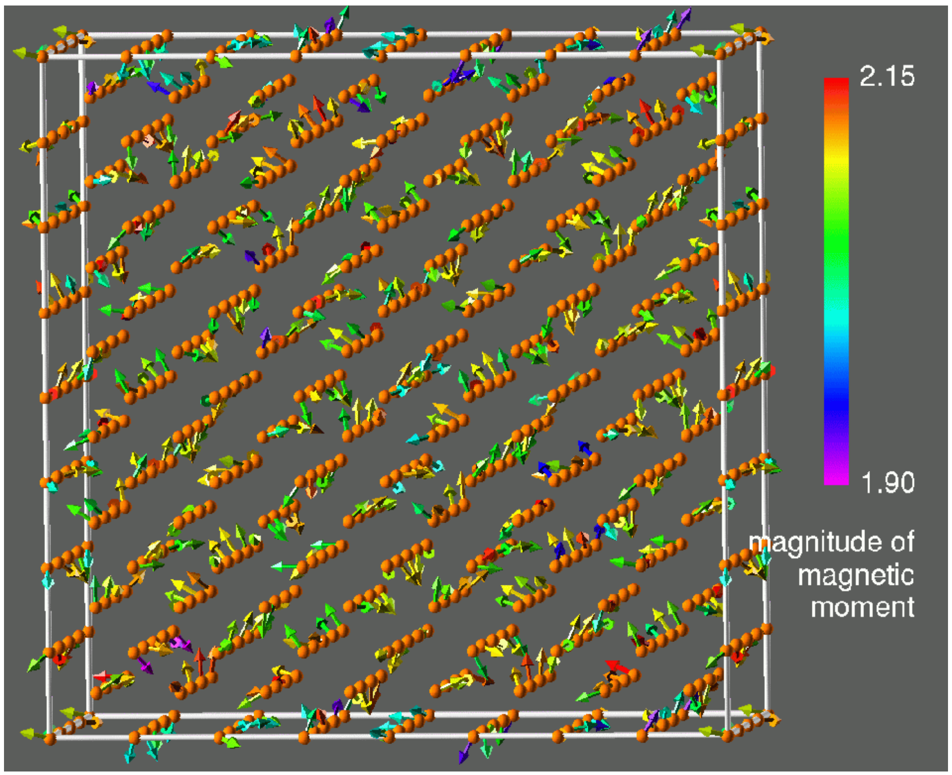
## *Future Plans*

Recompete Scientific Application Partnerships

Closer Partnerships with Program Offices

# Advancing Materials Sciences

## Understanding the magnetic properties of materials will enable the design of stronger, lighter magnets and new materials for magnetic data storage and recording.



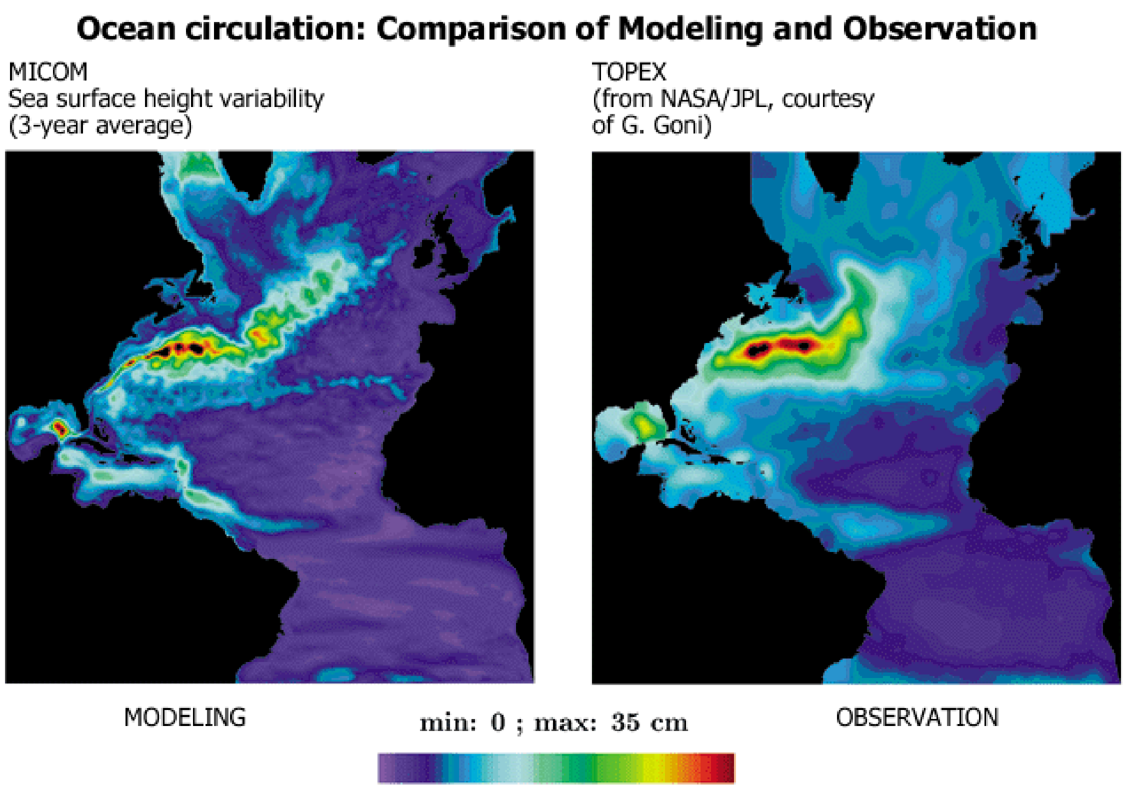

Scientists recently reported a break-through in calculating the magnetic properties of materials.

Combining modeling advances with the most powerful DOE-SC computer, DOE scientists were able to predict the effect of temperature on the magnetic moment of a crystal of iron. This is the first step to predicting the performance of magnets at typical operating temperatures.

*These simulations won the 1998 Gordon Bell prize in supercomputing for the fastest scientific application.*

# Advancing Climate Simulation

Climate simulation on terascale computers will improve our understanding of global climate and enable the study of regional scale impacts of global change.




DOE's program is an element of the U.S. Global Change Research Program.

DOE's program is designed to make full use of the computing capabilities provided by computers capable of 10 to 100 teraflops.

The new program will provide greater certainty in predictions of future climates at both global and regional scales. It will also provide detailed information on the effects of climate change, including many not now possible, *e.g.*, changes in topical storm frequency.

# Collaboratory Tools & Pilots
# FY 2000: $7M

## Vision & Objectives

Accelerate the ability of DOE to accomplish its mission through advanced computing and collaboration technologies.

## Accomplishments


**Tomographic Analysis**


Telepresence Collaboratories Enable Access to DOE Resources via the Internet

## Ongoing Projects and Applications

### National Collaboratories

Materials Microcharacterization Collaboratory

Diesel Combustion Collaboratory

R&D technology projects

### Grand Challenge and other projects

Supercomputer Solution of Massive Crystallographic and Microtomographic Structural Problems

Applications-Network Technology-Network Testbed Partnerships

## Future Plans

Award new/renewed NC projects with increase emphasis on

- Coupling R&D with pilots
- Collaborative Problem Solving Environments
- Grid-enabled applications

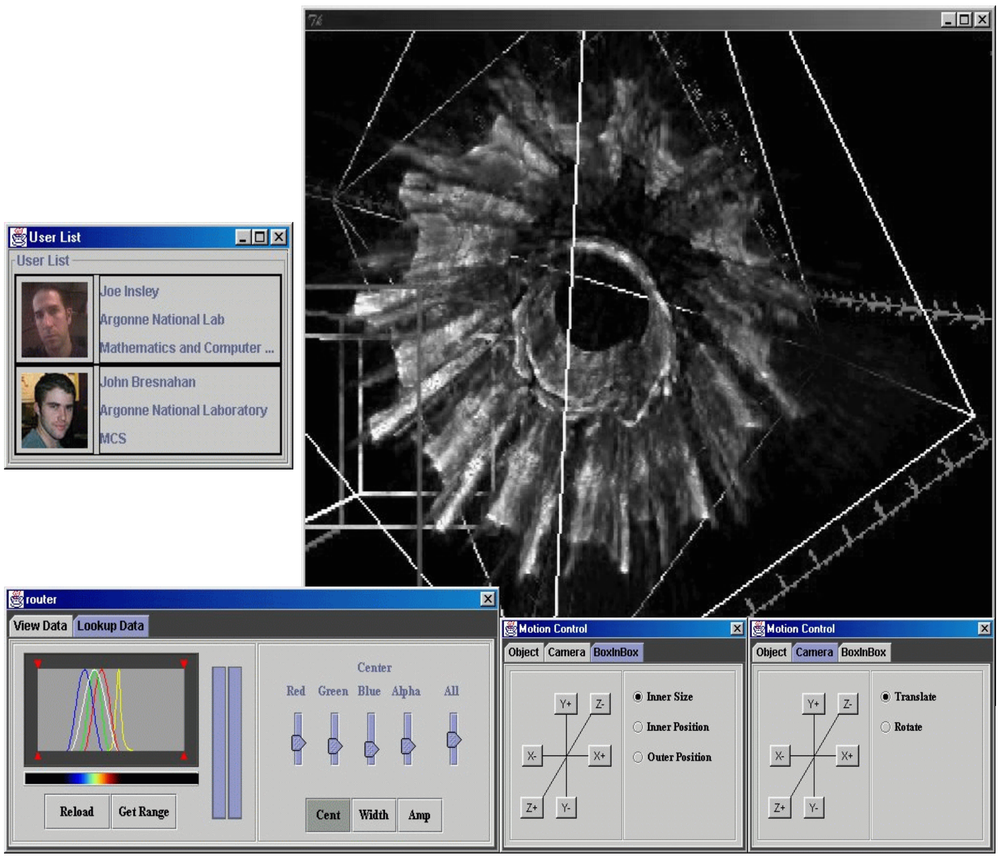
**2001** **2002**

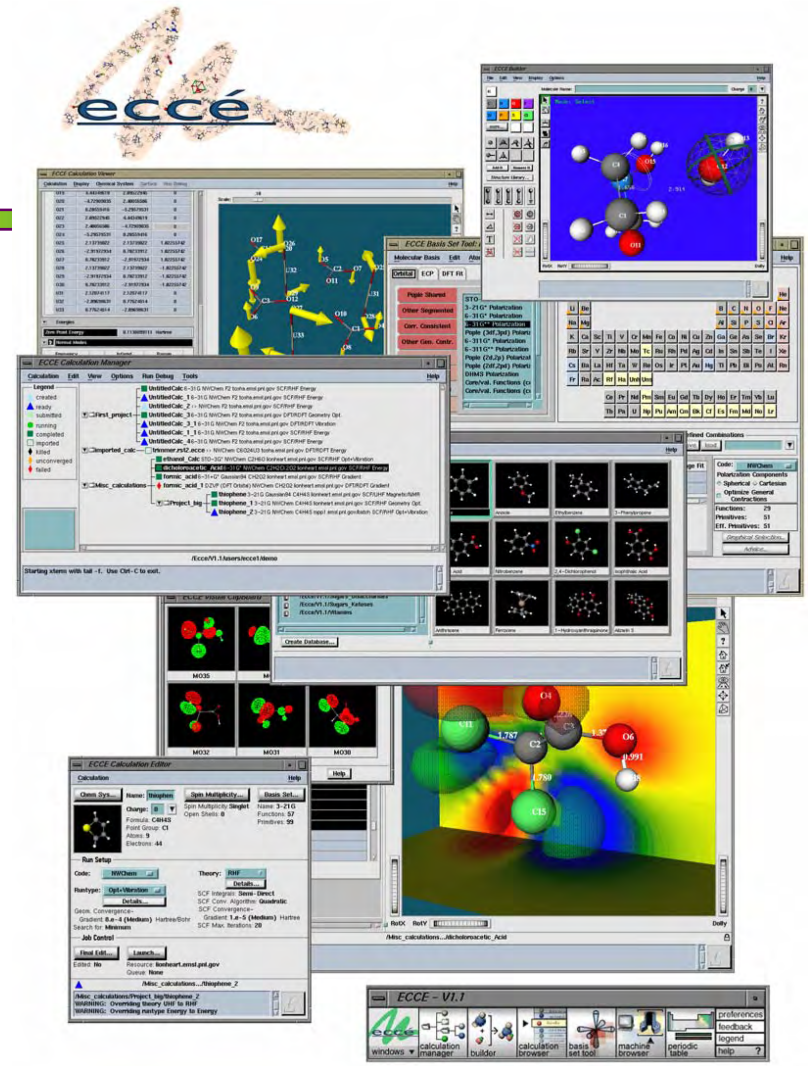
# National Collaboratories - Headline Success Stories

- Remote Operation Of Unique Instrumentation Can Speed Up Research
- TelePresence to the Rescue: Medical Emergency at the South Pole
- Collaboratories Are Influencing Industry Directions
- Real-time Reconstruction of Microtomographic Data Becomes Possible
- Going Paper-Free in the Clean Room
- The Particle Physics Data Grid is Paving the Way for Distributed Analysis of Future High Energy Physics Experiments
- PNNL Comes to You: Enhancing Science Education at Eastern Oregon University
- Remote Instrument Operation Works Internationally
- Virtual NMR Facility Matures into Core Resource at National Scientific User Facility
- Extending the Learning Experience by Bringing TelePresence Microscopy and Science Collaboratories into the Class Room

# Early Examples of Grid Applications

Quasi-real-time, collaborative supercomputer analysis of microtomographic data




Access to remote supercomputers from desktop interfaces

# High-Performance Network Research Program FY 2000: $2M

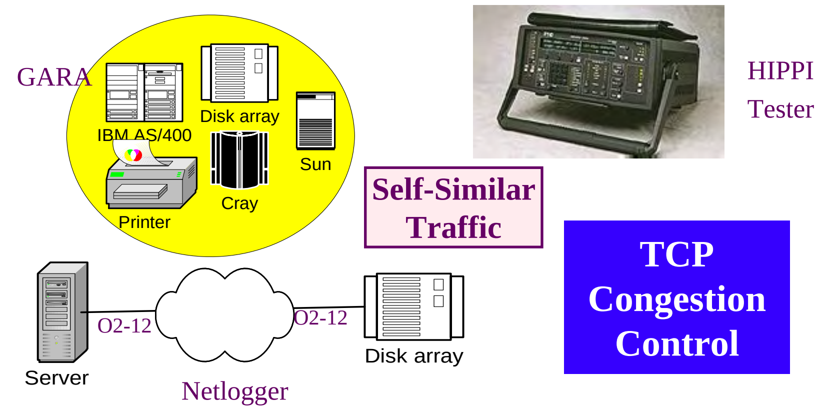
## Goals and Objectives

To develop secure and scalable high-performance networks to support wide area distributed high-end applications, the science grid, and collaboration.

To accelerate the adoption of emerging network technologies into production networks through testing and advanced deployment.

To provide leadership in the research and development of advanced networks services that have direct impact on DOE mission.

## Accomplishments




## Program Elements

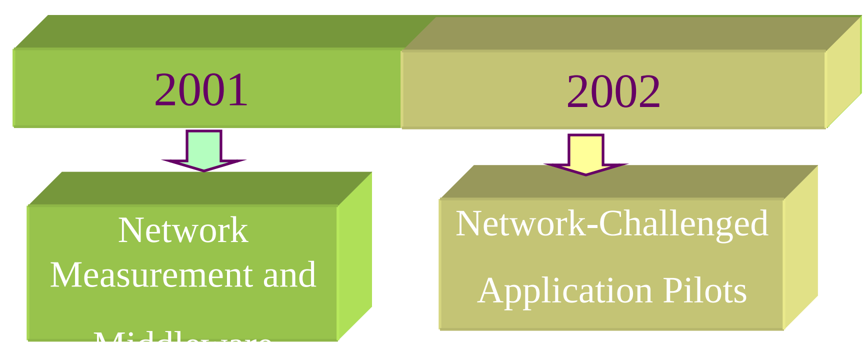
Traffic Modeling and Simulation

Network-Aware Middleware

Traffic Modeling and Simulation

Intelligent Network Security

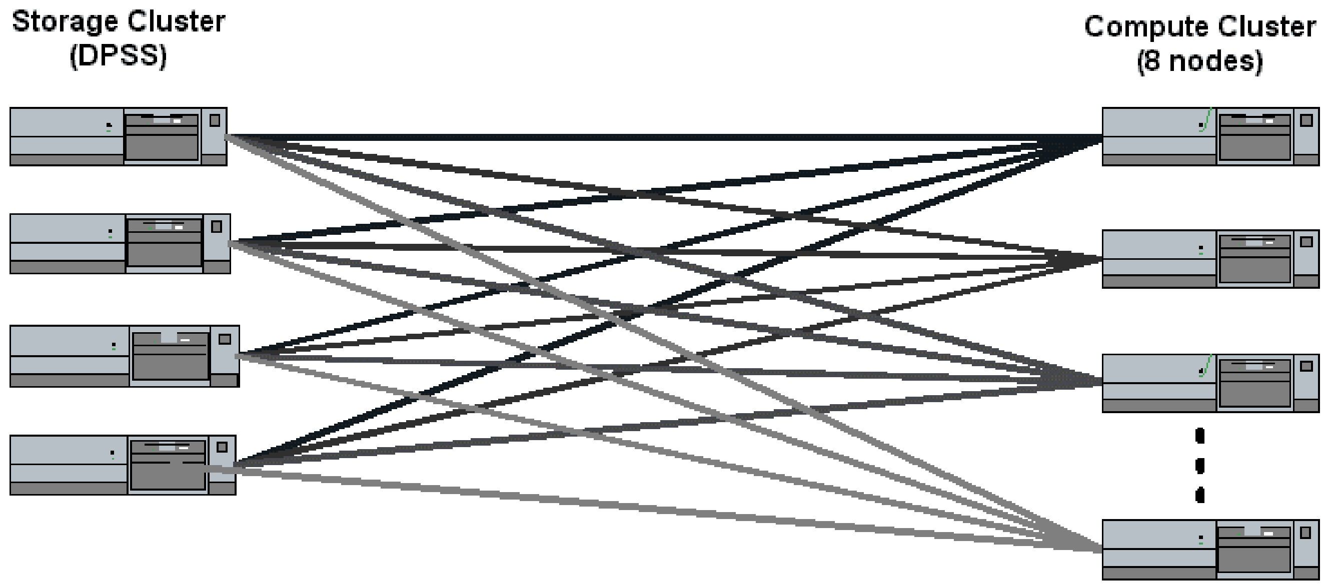
## Future Plans



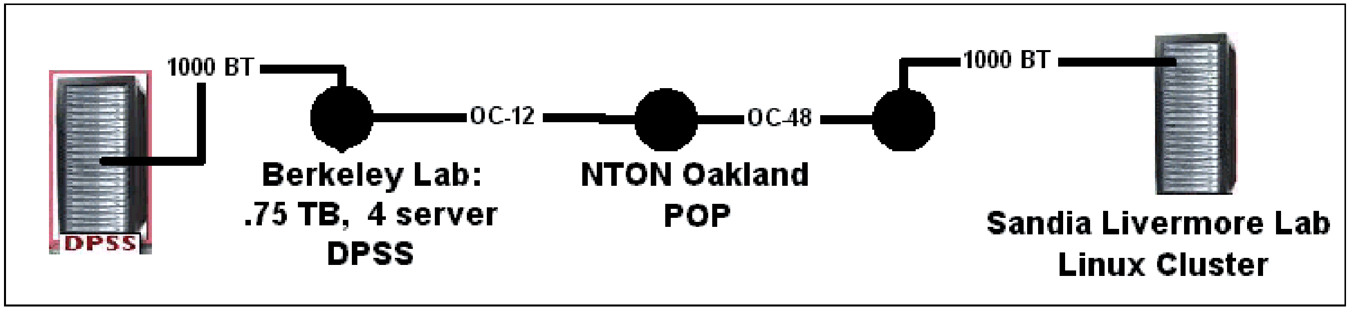
# Distributed Parallel Storage System (DPSS)

The DPSS is a collection of disk servers which operate in parallel over a wide area network to provide logical block level access to large data sets. To achieve high performance they exploit many levels of parallelism, including that available at the level of the disks, controllers, processors / memory banks, servers, and the network. DPSS has achieved 570Mb/sec over an OC 12 Connection.

# Distributed Parallel Storage System (DPSS)




Total Throughput = 570 Mbits/sec ( 71 MB/sec) on 32 data streams, or 17 Mbits/stream



# High Performance Computing and Communications Facilities

- High Performance Computers for Scientists (NERSC)
- High Performance Networks to Support Scientific Research (ESnet)
- Testbeds to Support Computational Science and Computer Science Research (ACRF’s)

# National Energy Research Scientific Computing Center (NERSC)
# FY 2000: $26.5M

## *Goal/Objective*

Provide Capability Resources and Professional User Friendly Services to Computational Scientists on Projects within the Missions of the Department of Energy

## *Accomplishments*

- Gordon Bell Prize winning Magnetic Materials effort: First over 1 Tflops
- Parallel Climate Model: T3E@17GFlops
- Accelerator Design and Modeling: SNS
- Turbulent Transport in Tokamak Core
- Boomerang (Our Universe is Flat!)
- Quantum Chemistry: Electron Scattering off Hydrogen

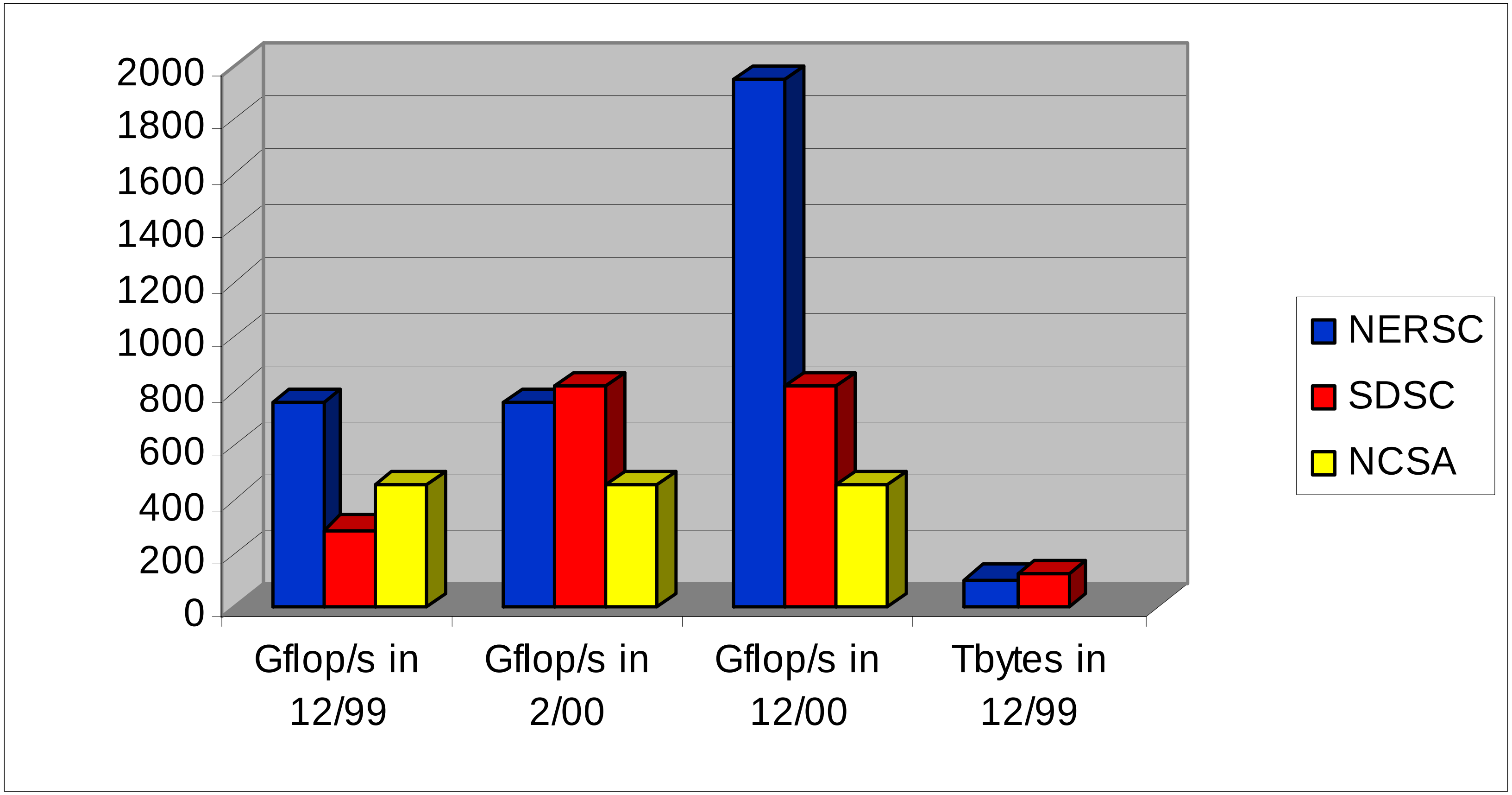
## *Program Elements*

- Operations of HPC's: J-90 PVP, T3E MPP, and IBM; Storage: HPSS
- Advanced Systems and User Services
- HPC Research including Future Technologies

## *Future*

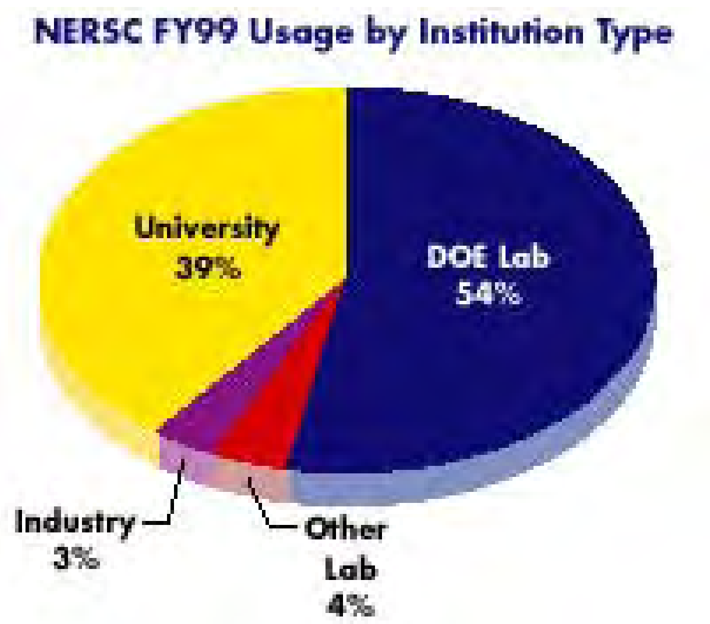
- Near Term: Again the world's most powerful unrestricted computing center at ~3.0 TeraFlops
- Nearer Term: Move Hardware and Operations to the Oakland Building

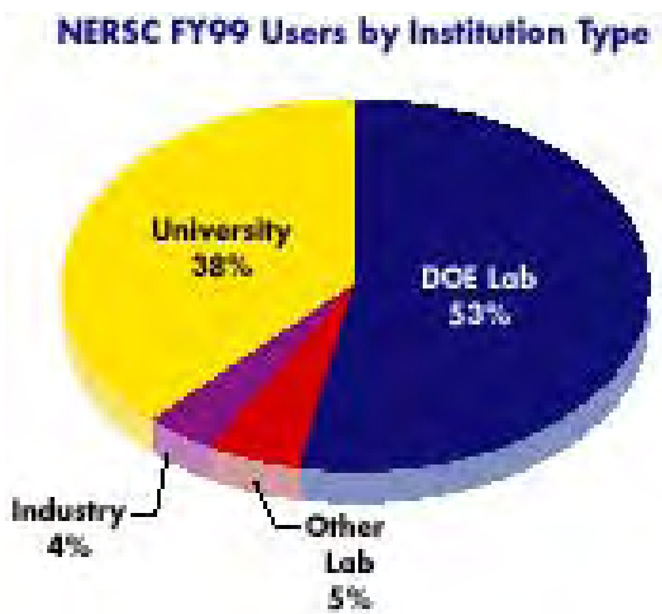
# NERSC Facility: Comparison to Similar Centers in the U.S.




**Gflop/s based on R_max value of machines as published in the TOP500 list**
**Tbytes based on total amount of file storage in HPSS systems**

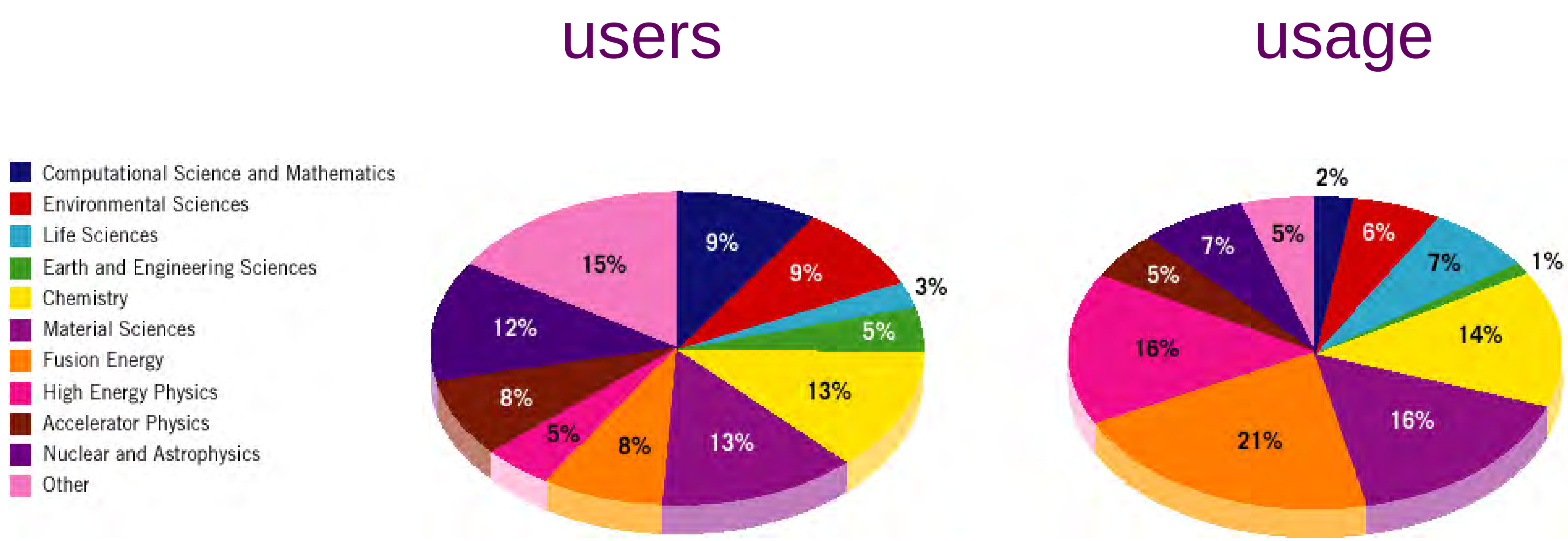
# FY 1999 Allocations



# NERSC Serves a Broad Array of Disciplines

## FY 1999 Distribution



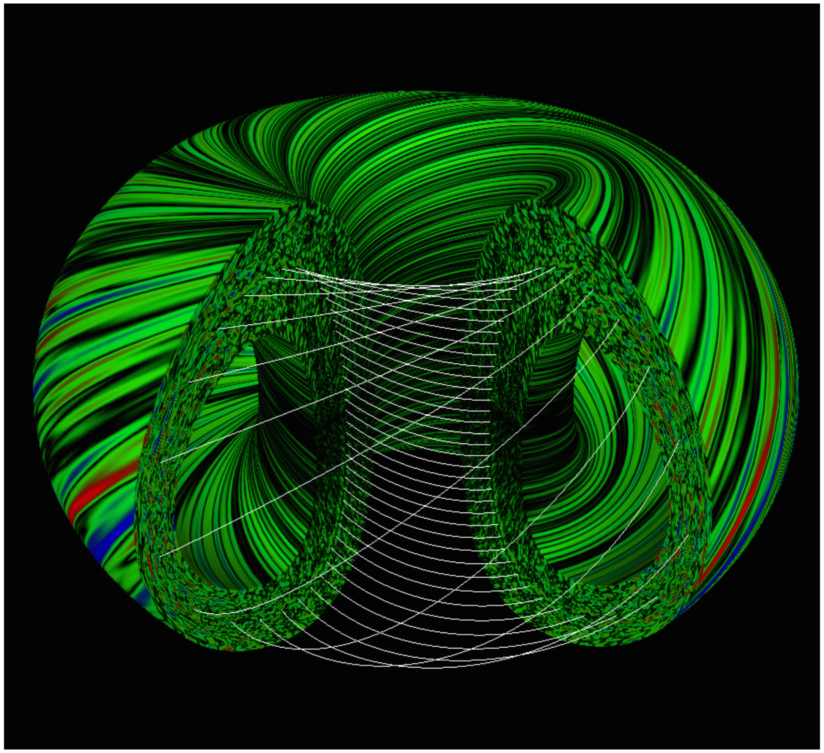
# Computational Science Enabled by NERSC

NTTP Grand Challenge:

- unprecedented progress in understanding turbulent transport in tokamak core plasmas
- more than 60 publications based on NERSC results

Bruce Cohen, LLNL, about NERSC:

"… **All but a very small percentage of these results were obtained on the T3E at NERSC. Essential to obtaining these results on the T3E were the large memory (needed to support high resolution three-dimensional time-dependent calculations and good particle statistics in the kinetic calculations), the large number of processors, the high rate of availability, the excellent production environment (excellent mix of interactive and batch, excellent debugger and job scheduler, and consultants), and the big allocation that this project has enjoyed. "**



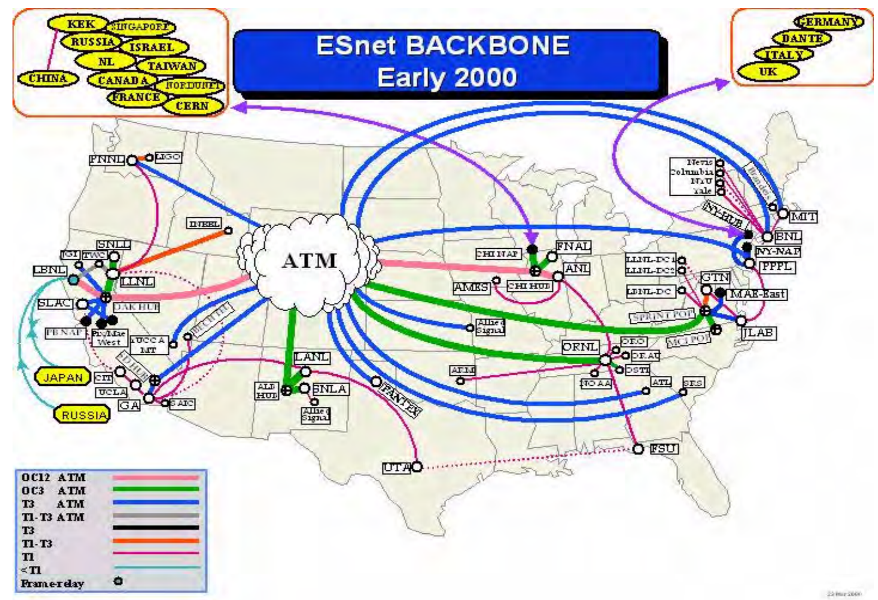
# ESnet FY 2000: $17 M

## *Goal:*

A future in which advanced network capabilities enable seamless collaborations for DOE and its researchers"

## *Objective:*

Provide highly capable and reliable communications infrastructure and leading-edge network services that support DOE's missions




## *Program Elements:*

- Nation-wide high-performance research network
- Advanced network services to support science in DOE
- Immense (and very successful) cooperative effort
- Extensive structure of domestic (commercial and R&E) and international interconnects
- Advanced Technology and Research program

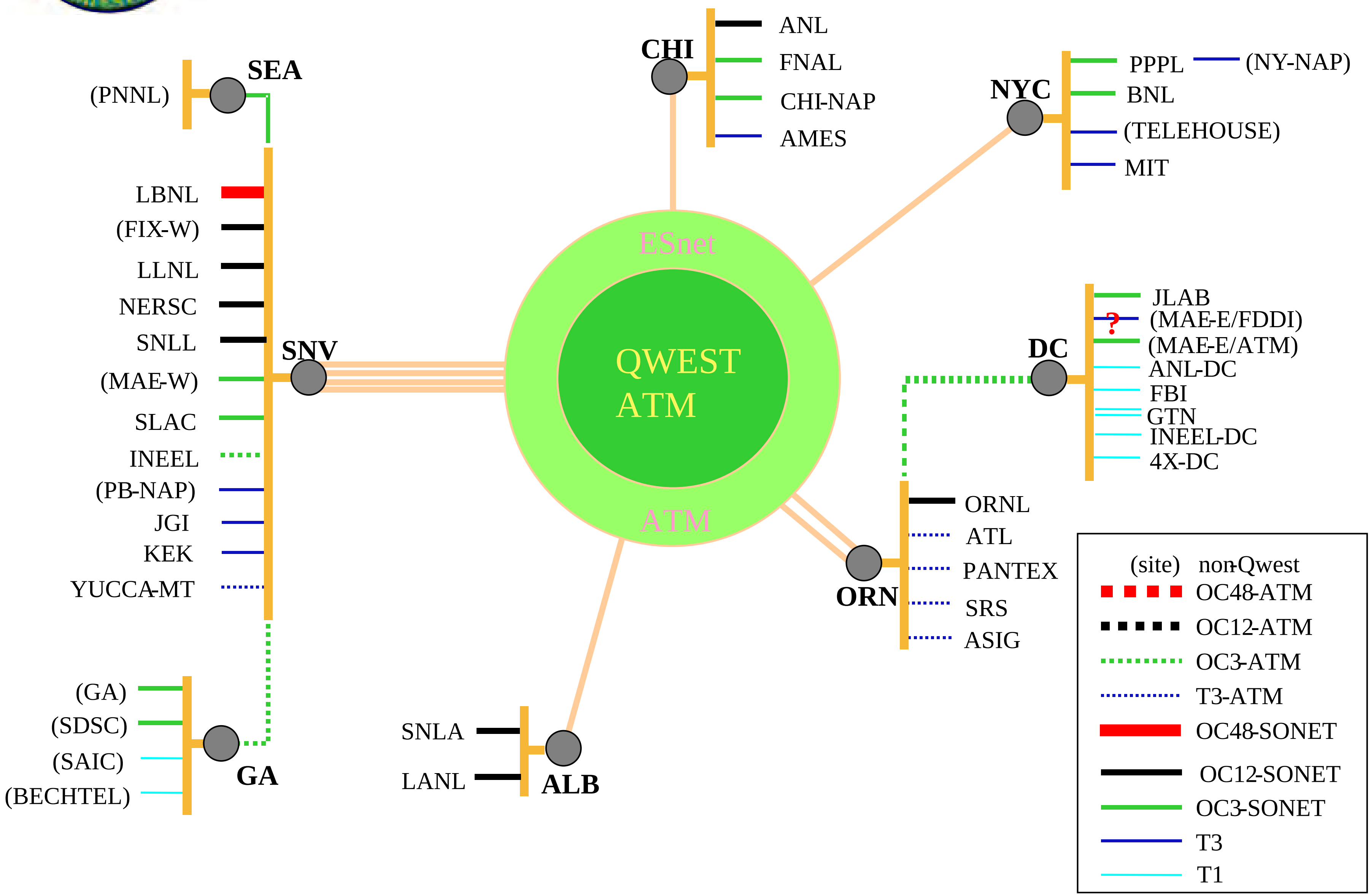
## *Future:*

- Continue to improve on success
- Research and implement new technologies
- Increase emphasis on research, security, and coordination with other Federal Network efforts
- Be an enabling component of the DOE collaborative and Grid environments
- Stay nimble and current with emerging technology

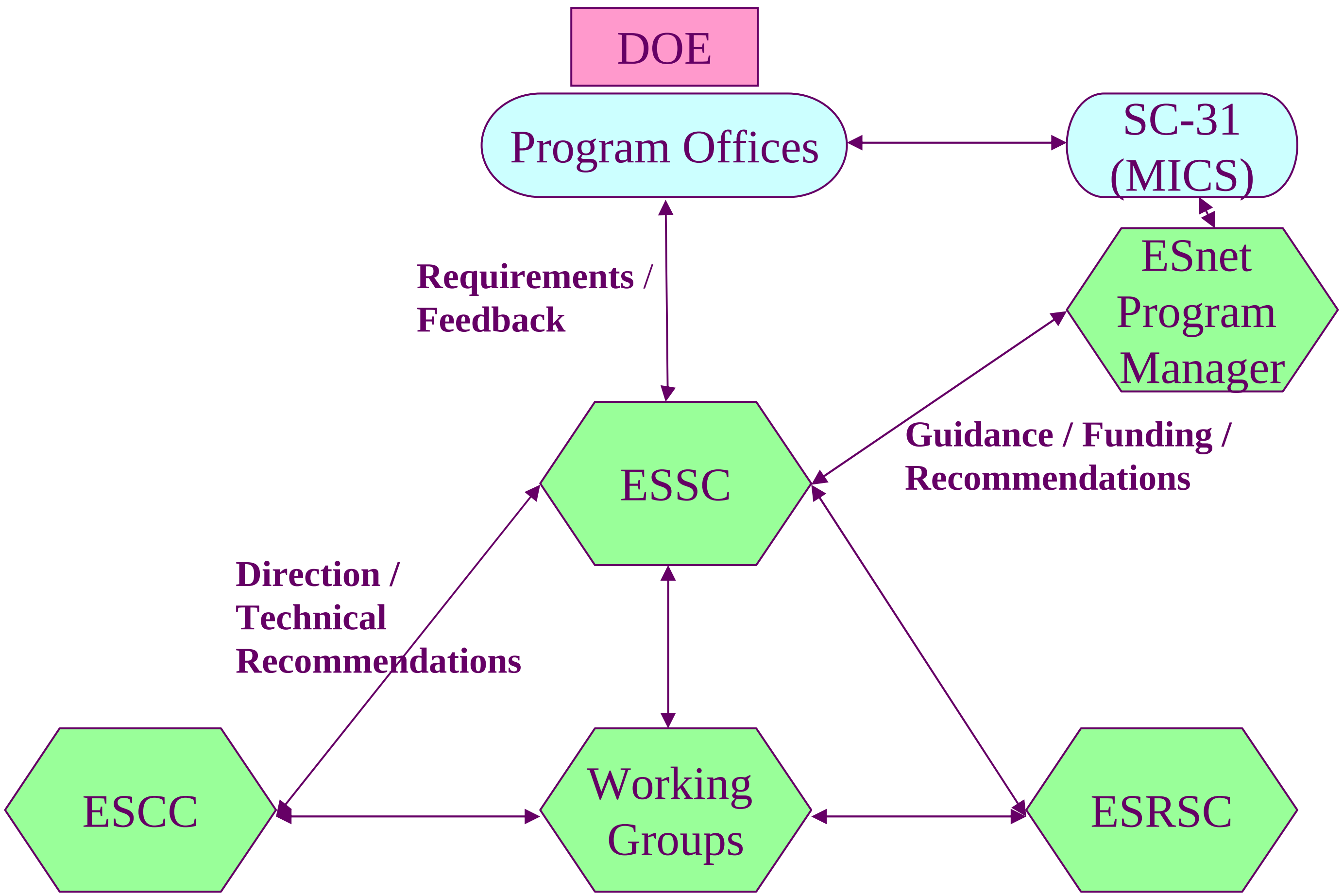
# ESnet - History

- Pre- HPCC: 1986 - 1991
  - ESnet declared to be the "official" network for all of Energy Research (now Office of Science - SC)
  - Backbone - a combination of 9.6K and 56K satellite and terrestrial circuits, DECnet & TCP/IP
  - 22 sites connected by end of 91 to T1 Backbone
- 1992-1994
  - Competitive RFP launched for "Fast Packet ESnet Services"
  - '94 Contract Awarded to Sprint T3 and up
- 1995 - 1999
  - '95 ESnet Operations re-competed, moved to LBNL
  - Traffic grows from 2.4 to over 8.7 Tbytes/month & T3 and OC3c ATM based interconnects established
- 2000 ESnet: new contract with Qwest: *Beyond ATM*

# ESnet INITIAL Qwest CONFIGURATION



# ESnet Program - Committees



# Advanced Computational Research Facilities FY2000: $11.5M

## Objectives

Provide pioneer capability computing for scientific applications relevant to the Office of Science mission.

Provide Testbeds to examine critical CS issues

## Accomplishments

Provided state-of-the-art computational resources for Grand Challenge calculations.

Evaluated feasibility of innovative computer architectures (IBM SP, SGI Origin 2000, Paragon) to meet SC computational needs.

## Ongoing Projects

CHIBA City, a 512 CPU Linux cluster (ANL).

Falcon & Colt - Compaq AlphaServer SCs (ORNL).

Nirvana, 2048 Processor SGI (LANL)

“Probe” HPSS Testbed (LBNL/ORNL)

TERA Evaluation- (UCSB)

Prototype Topical Center(ORNL)

## Plans

Explore novel architectures & testbeds

Evaluate for topical applications

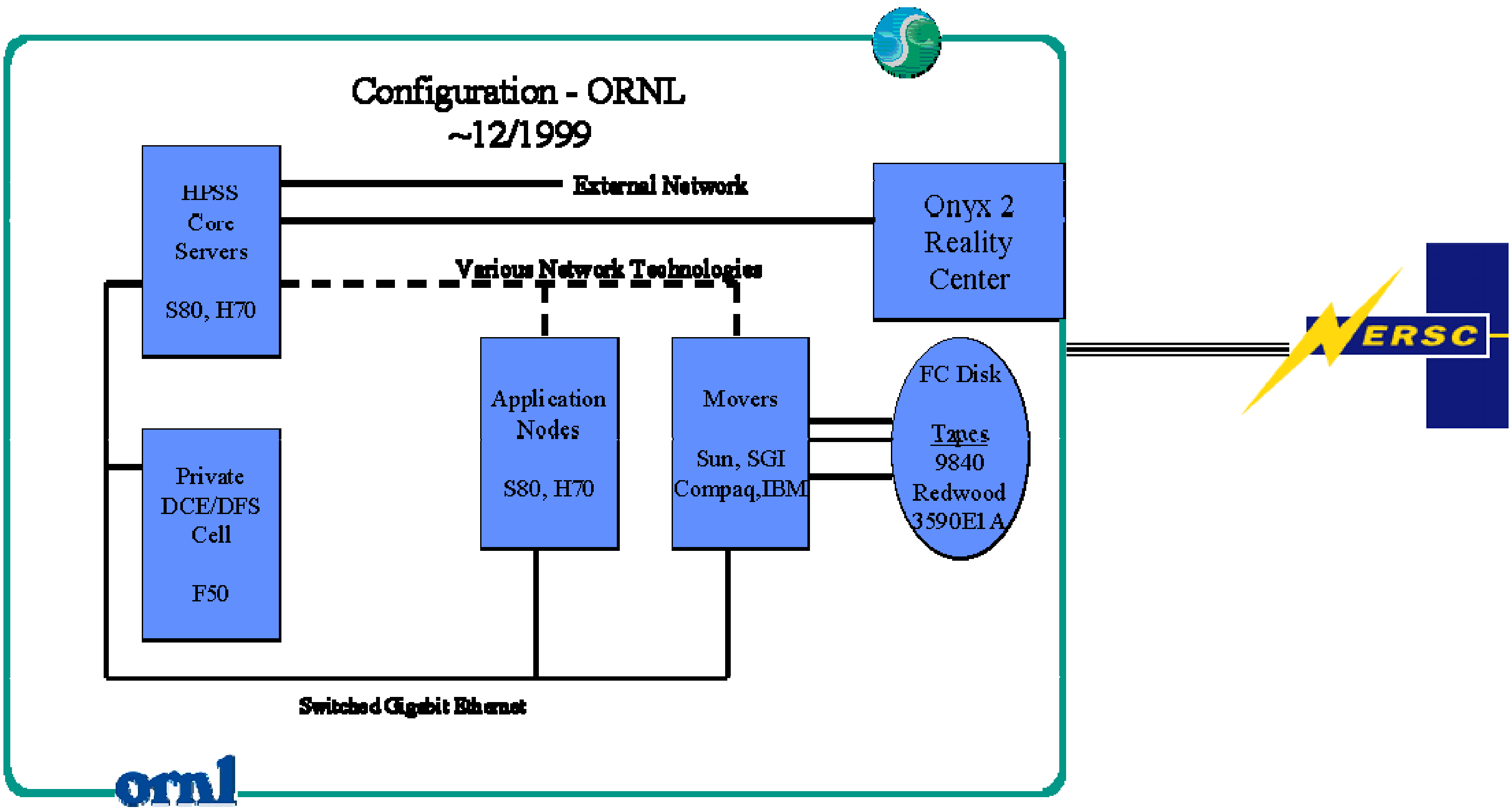
Expand technical & vendor bases for future hardware purchases.

# ACRF Evolution

- High Performance Computing Research Centers
  - FY1992-  Established High Performance Computing Research Centers at LANL & ORNL (global climate/ground water).
  - FY1993- Initiated Grand Challenge computational research program.
  - FY1995- Established an HPCRC at ANL (applications testing/computer science).
- FY1995-2000- Advanced Computing Research Facilities
  - Upgraded hardware at LANL
  - Focused ORNL and ANL efforts toward research.
  - Coupled Grand Challenges to specific HPCRC.
  - Allocated portion of NERSC allocated for Grand Challenges.
- FY 2000- Completed Grand Challenges.

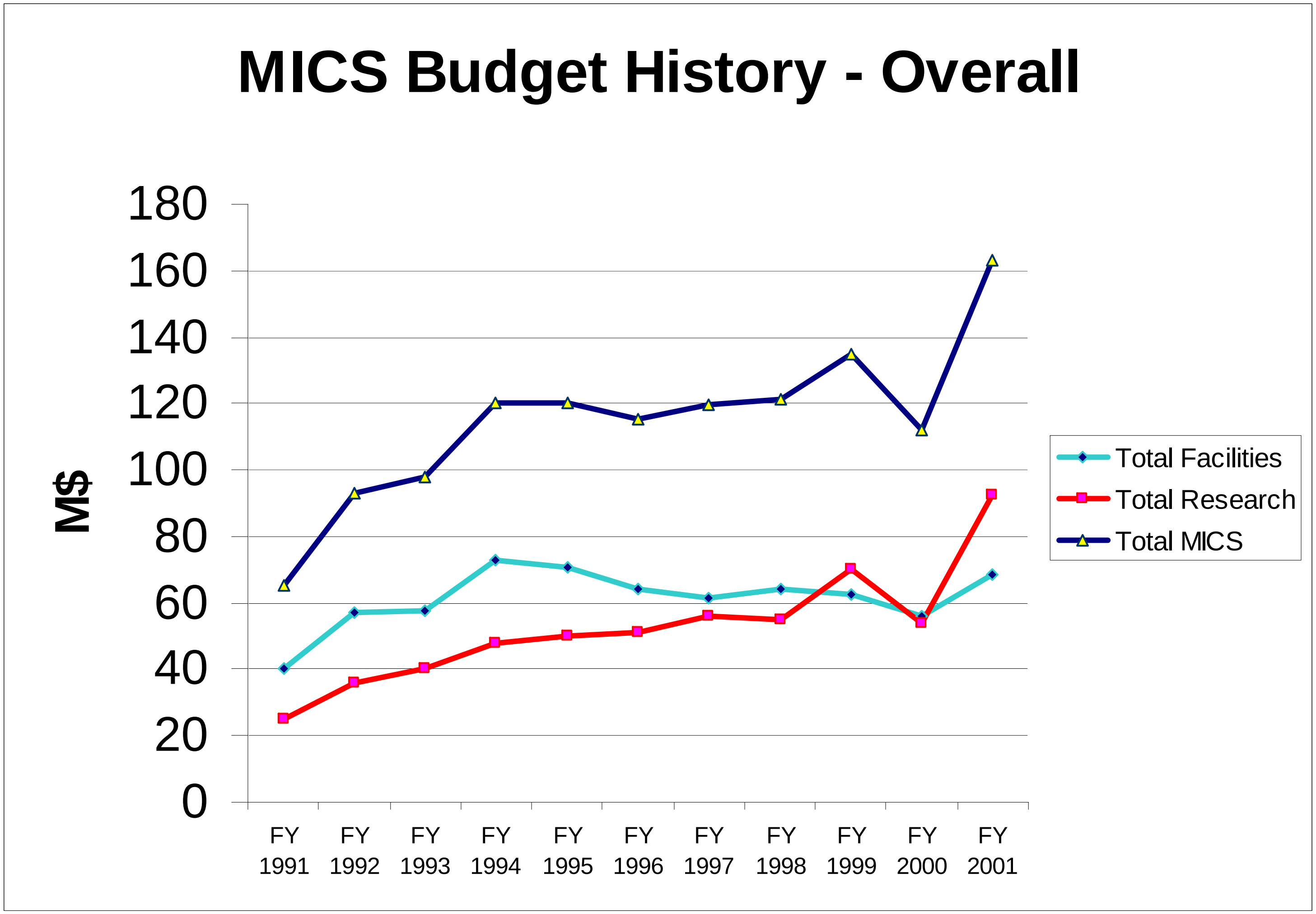
# Probe Testbed

Enable Research on Terascale File Storage and Data Systems

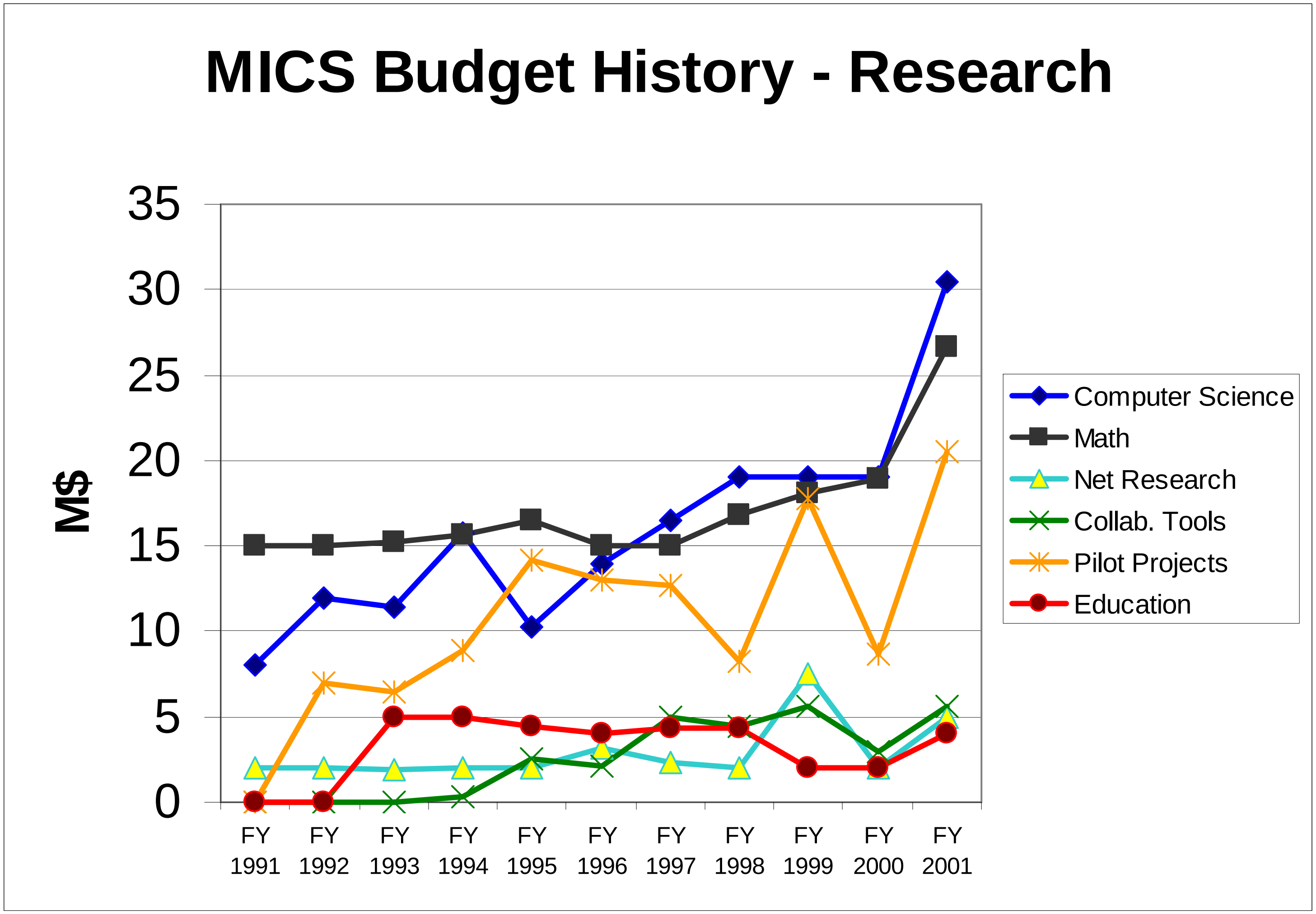


# Budget Detail Backup

# MICS Budget History

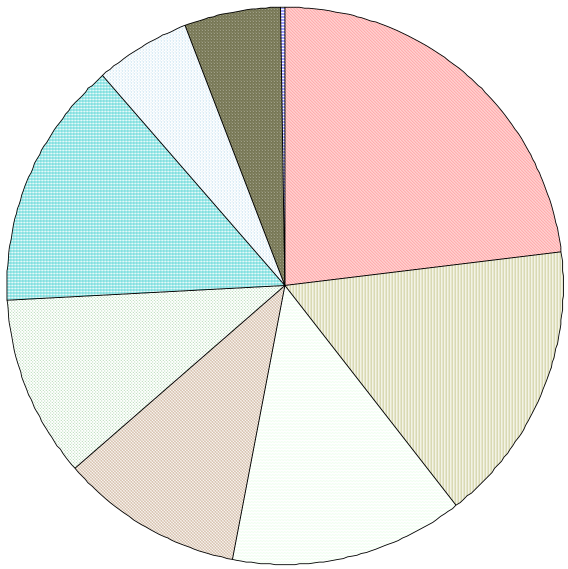


# MICS Budget History

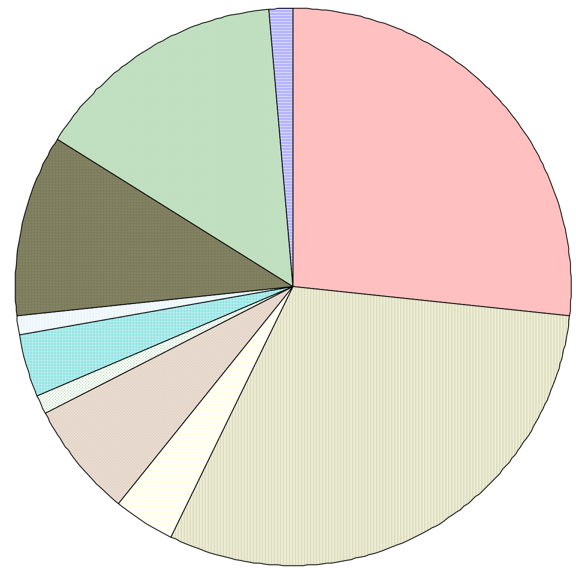


# Distribution of Applied Math Research Projects

## FY 2000 Labs: $14.0M



## FY 2000 Universities: $5.1M

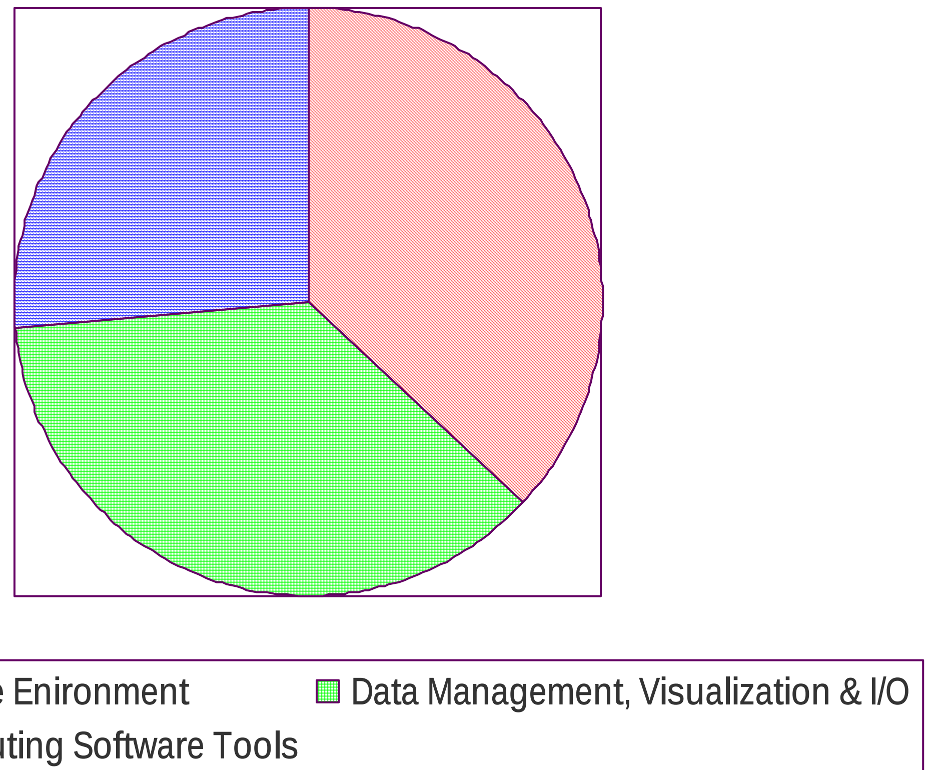


- Computational Fluids
- Differential Equations
- Linear Algebra
- Optimization
- Predictability
- High Performance Computing
- Mesh Generation
- Other
- HBCU
- Conferences

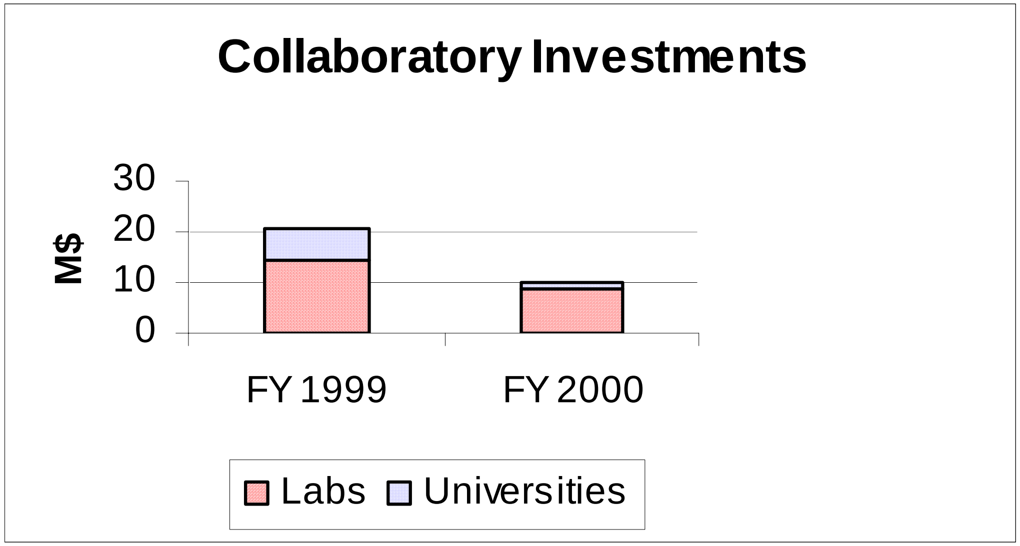
10-10-2000

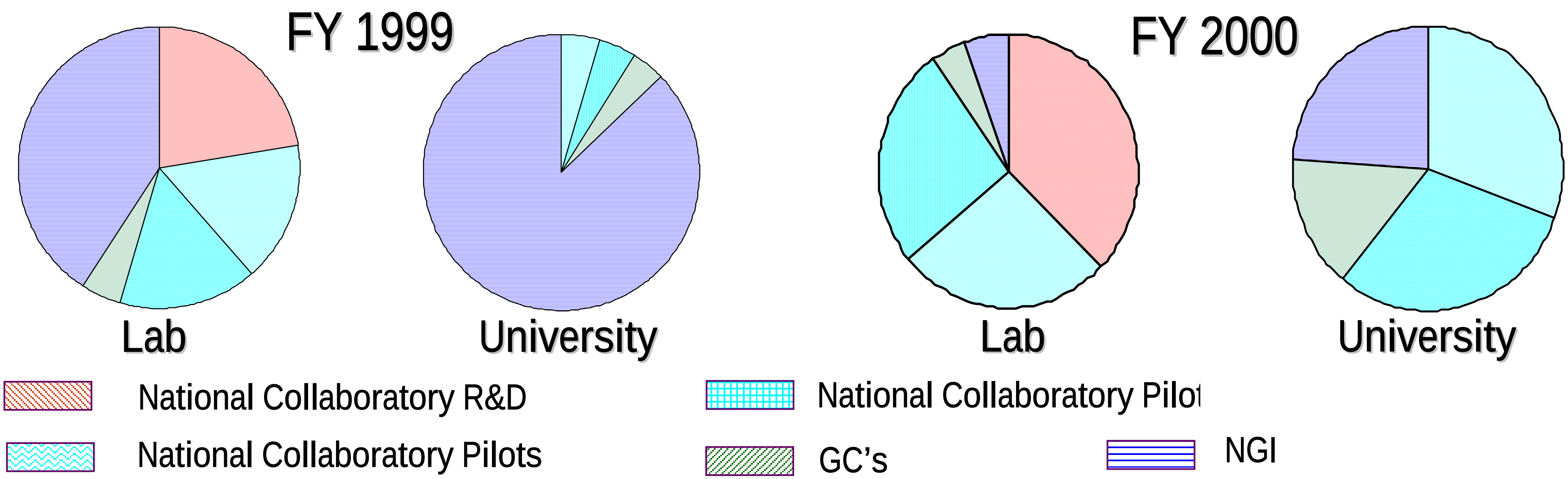
# Distribution of Computer Science Research Projects

## FY 2000 Labs: $15.2M      FY 2000 Universities: $3.8M



# Distribution of Collaboratory Projects



# Distribution of Network Research Projects