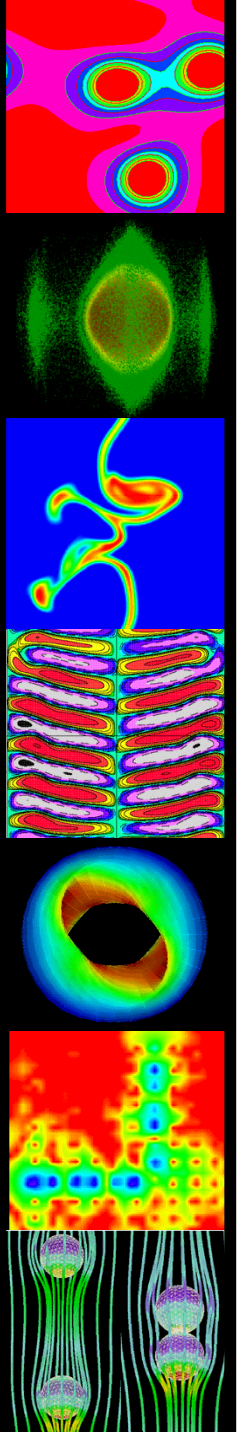
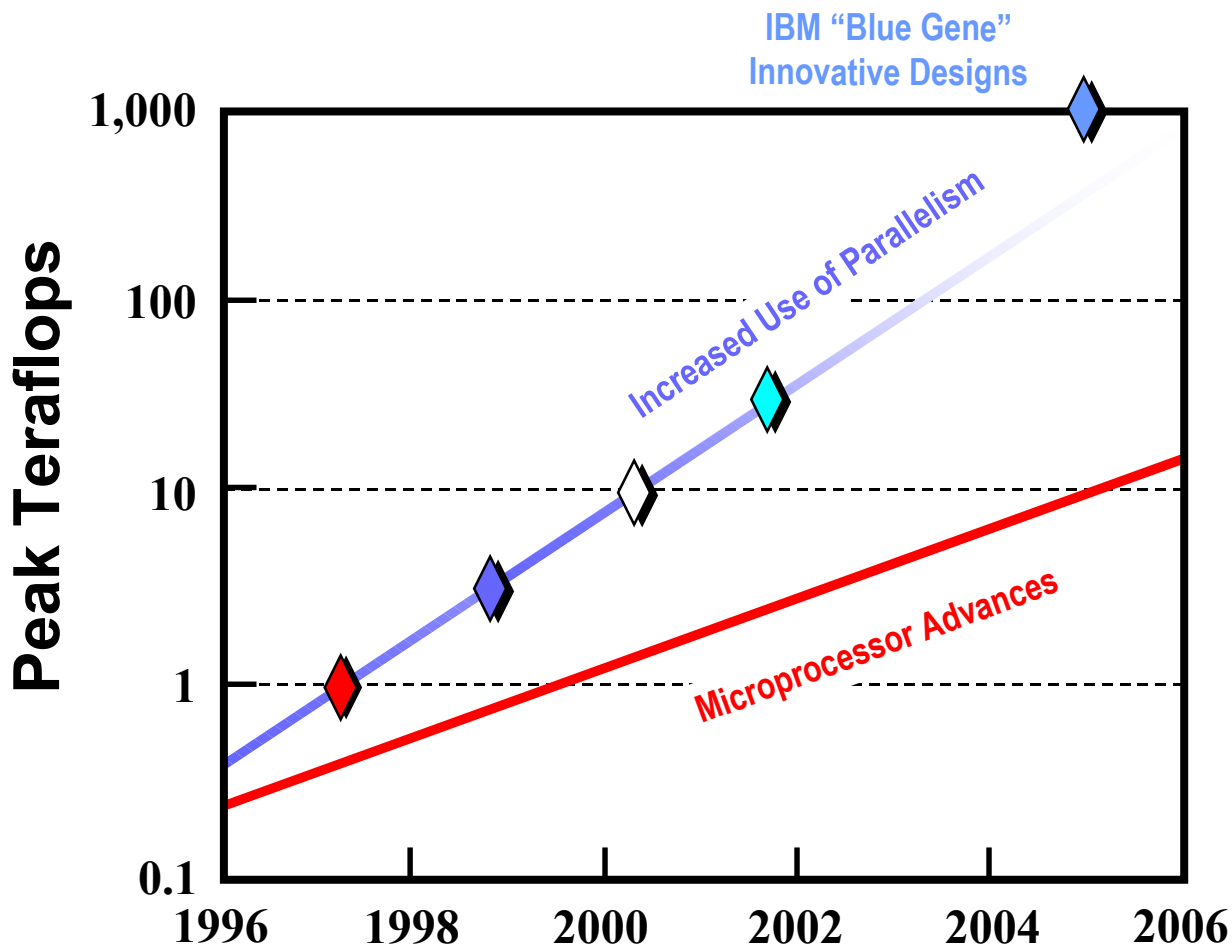


# Scientific Discovery through Advanced Computing

**Thom H. Dunning, Jr.**

**Assistant Director for Scientific Simulation**
**Office of Science**
**U.S. Department of Energy**

# Dramatic Advances in Computing
## Terascale Today, Petascale Tomorrow




**MICROPROCESSORS**

2x increase in microprocessor speeds every 18-24 months ("Moore's Law")

**PARALLELISM**

More and more processors being used on single problem

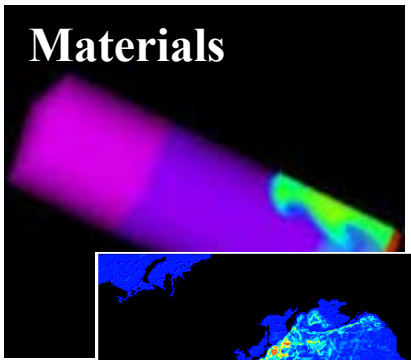
**INNOVATIVE DESIGNS**

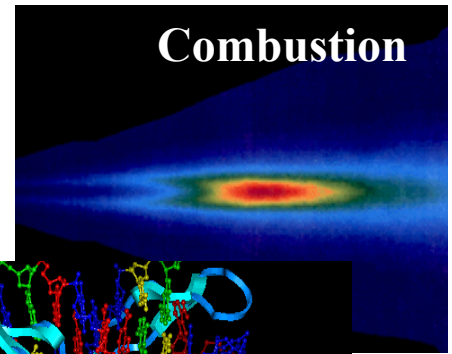
Processors-in-Memory
HTMT

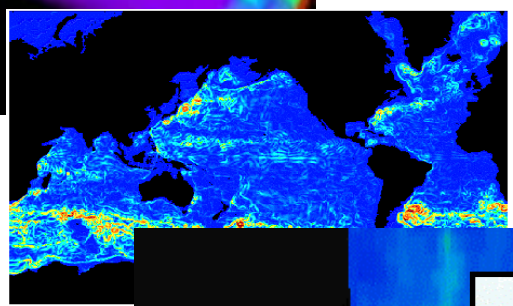
# Scientific Computing

## Critical to Discovery in Many Scientific Disciplines

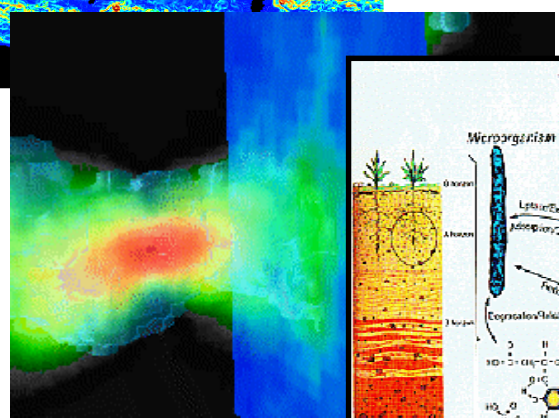
**Many SC Programs Need Dramatic Advances in Simulation Capabilities To Meet Their Mission Goals**



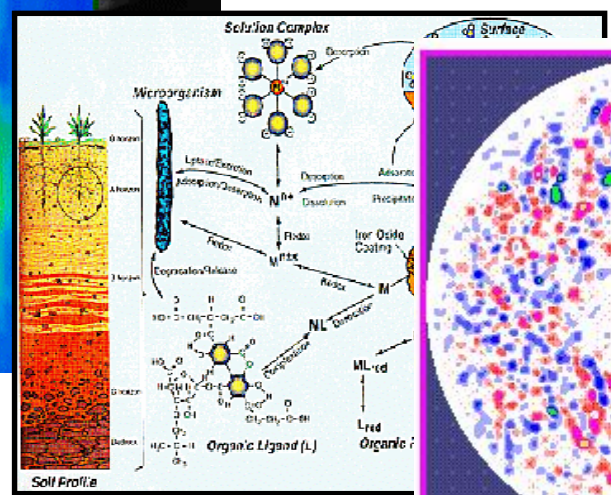



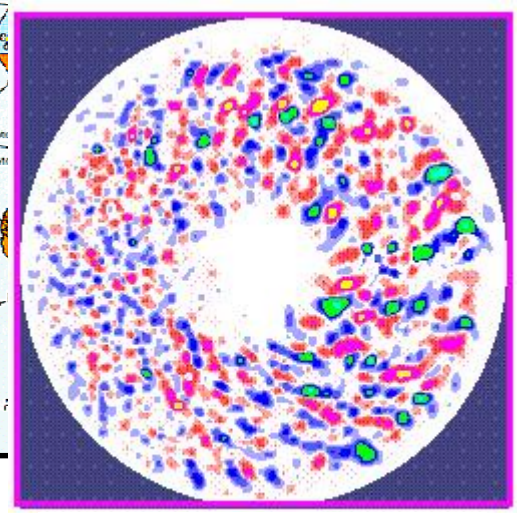
Global Climate



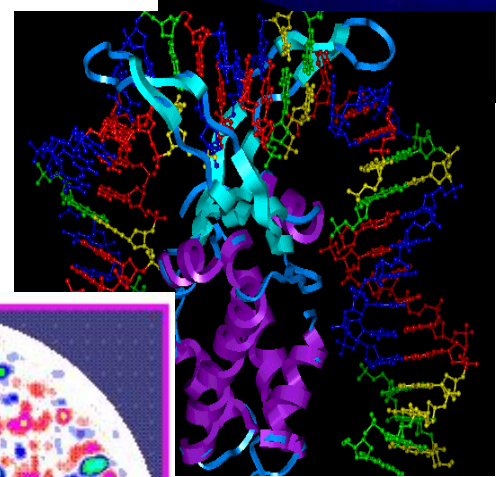
Components of Matter




Subsurface Transport



Fusion Energy



Health Effects, Bioremediation

# Goal and Strategies

## "Scientific Discovery through Advanced Computing"

- **Goal**
  - Promote scientific discovery throughout the Office of Science by exploiting advances in computing technologies
- **Strategies**
  - Create *Scientific Computing Software Infrastructure* that takes full advantage of terascale computing capabilities for scientific research
  - Establish *Scientific Computing Hardware Infrastructure* that supports scientific research in the most efficient, effective manner possible
  - Enhance collaboration and access to facilities and data through advances in networking technologies and development of electronic collaboratories

# Programmatic Elements

"Scientific Discovery through Advanced Computing"

## Hardware Infrastructure

## Software Infrastructure

OPERATING SYSTEM

COLLABORATORIES

DATA GRIDS

Data Analysis & Visualization

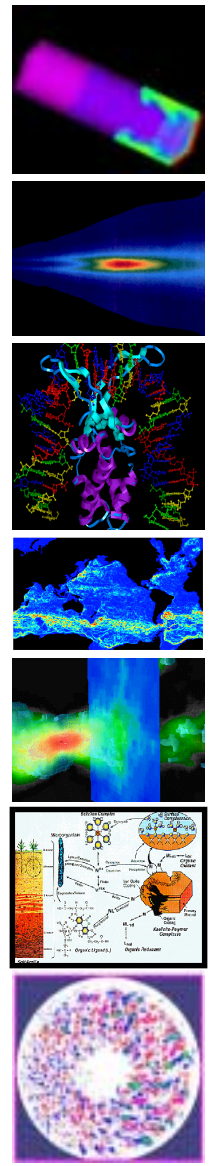
Mathematical Libraries

Programming Environments

Scientific Data Management

Problem-solving Environments

SCIENTIFIC SIMULATION CODES



ASCR

BES, BER
FES, HENP

# Scientific Computing Software Infrastructure

# SC Software Infrastructure
## A Major Software Challenge

### Peak Performance is skyrocketing

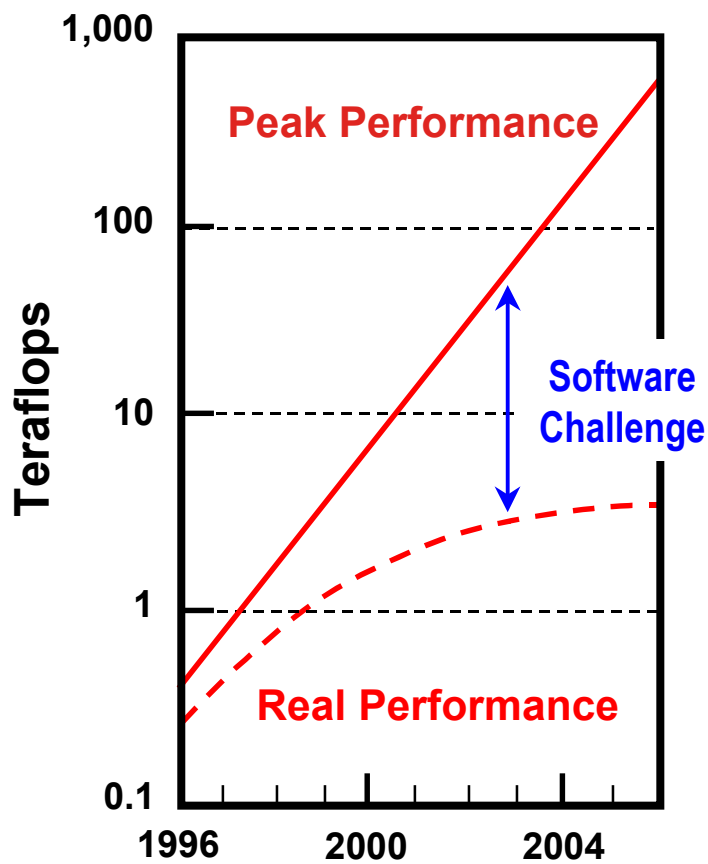
- In 90's, peak performance has increased 100x; in 00's, it will increase 1000x

### But ...

- Efficiency has declined from 40-50% on the vector supercomputers of 1990s to as little as 5-10% on parallel supercomputers of today and may decrease further on future machines

### Research challenge is software

- Scientific codes to model and simulate physical processes and systems
- Computing and mathematics software to enable use of advanced computers for scientific applications
- Continuing challenge as computer architectures undergo fundamental changes

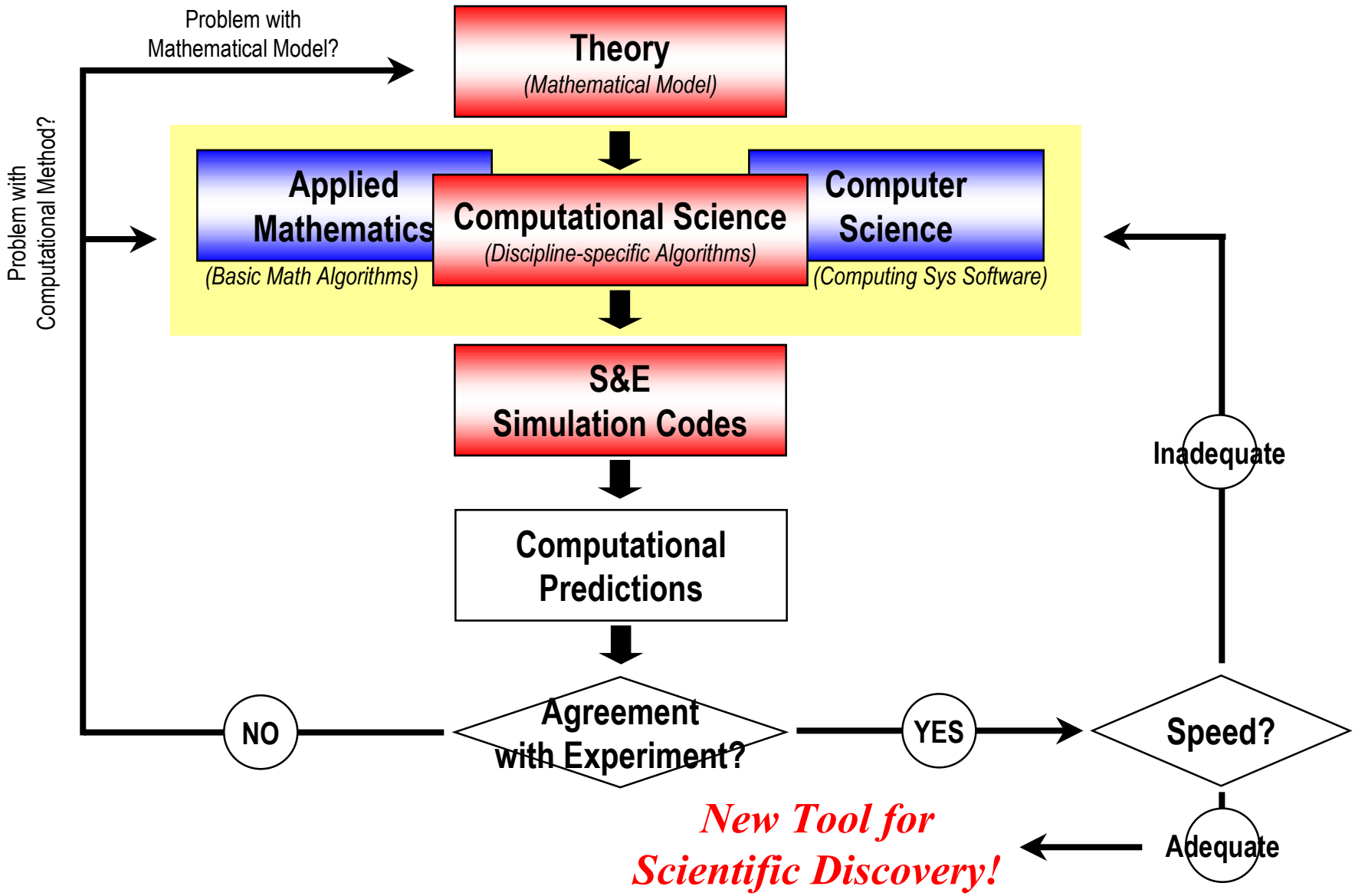


# Software Challenges
## Scientific Computing

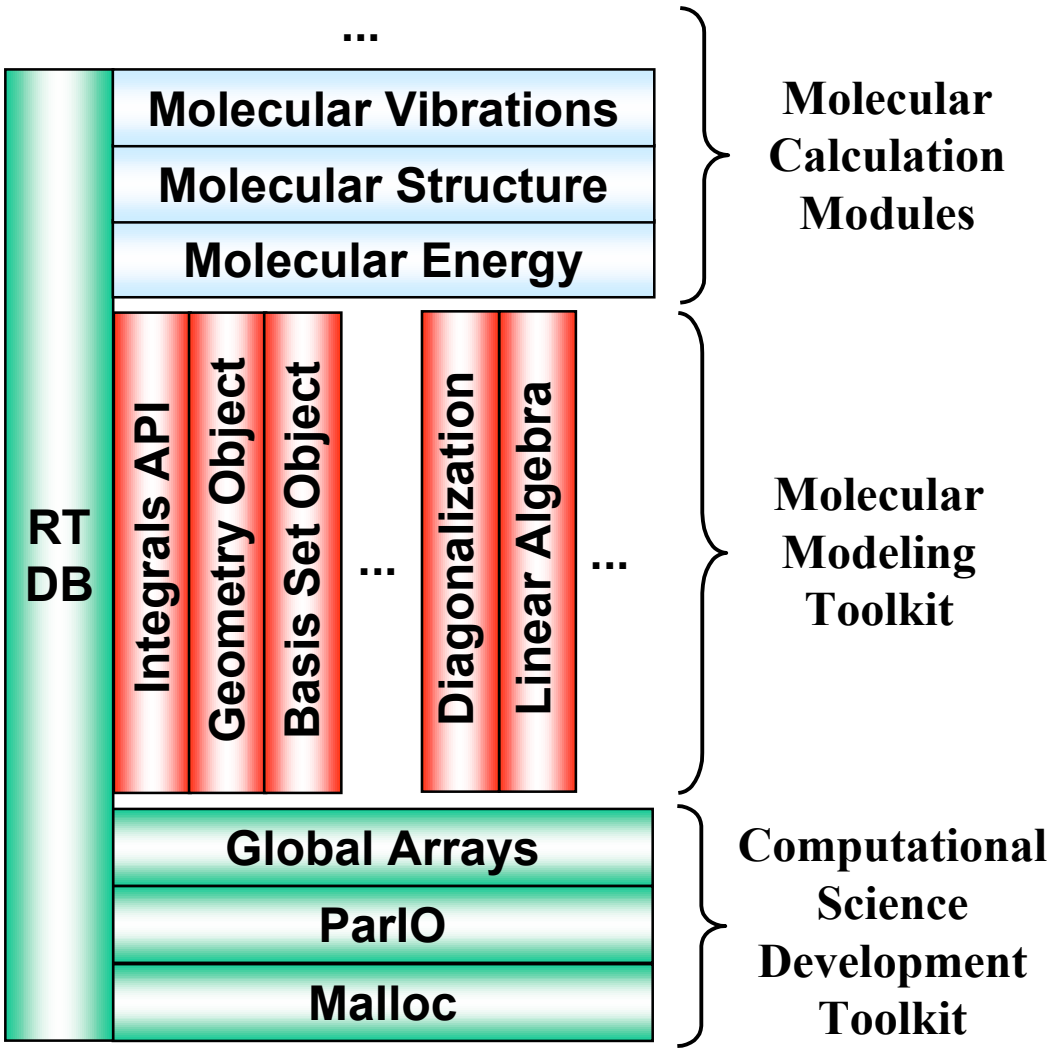
- **Scientific Codes**
  - High fidelity mathematical models
  - Efficient, robust computational methods and algorithms
  - Well designed computational modeling and simulation codes
    - Readily incorporate new theoretical advances
    - Port from one computer to another with minimal changes
- **Computing Systems and Mathematical Software**
  - Increased functionality in Vendor Operating Systems
  - Computing systems software
    - Accelerate development and use of terascale scientific codes
    - Facilitate porting of software and codes among high-performance computers
    - Manage and analyze massive ( petabyte) data sets, both locally and remotely
  - Algorithms that scale to thousands-millions processors

# SC Software Infrastructure

## Scientific Simulation Code Development Teams



# An Example
## Northwest Chem (NWChem)




## NWChem

*a major new modeling capability for molecular science*

Molecular Electronic Structure
Molecular Dynamics
(Crystals)
> 600,000 lines of code and growing

**Runs on ...**

Cray T3D/E, IBM SP2, SGI SMP, NOWs, Sun and other workstations, X86 PCs (Linux)

**Scales to ...**

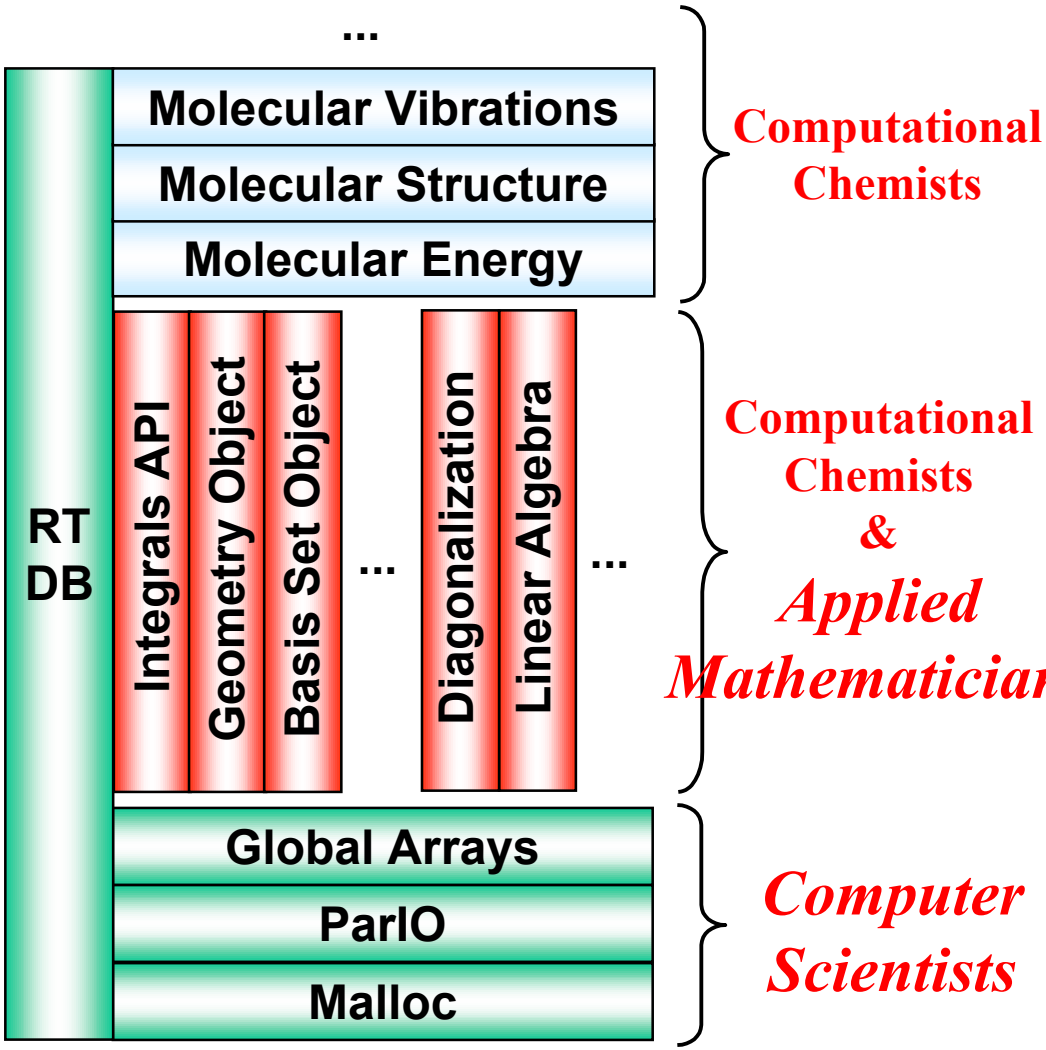
2,000+ processors

**Developers ...**

Core group (15) plus larger group (20) of world-wide collaborators
>100 person-years at PNNL alone

# NWChem

## Chemistry-Applied Math-Computer Science




**Molecular Modeling Toolkit**

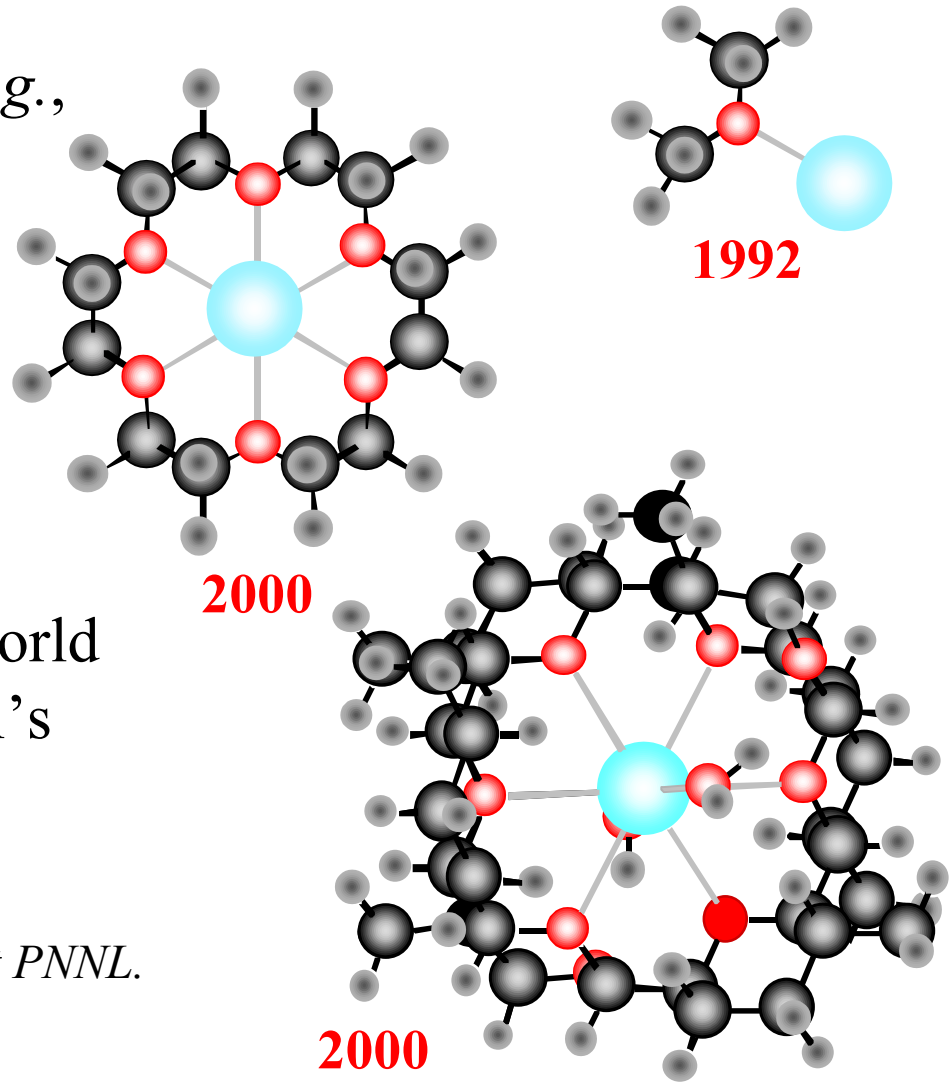
**Basic mathematical subroutine libraries.**

**Hardware Abstraction Layer**

**The only layer of NWChem that must be revised to make use of new computers. Only a small fraction of the code in this layer must be changed.**

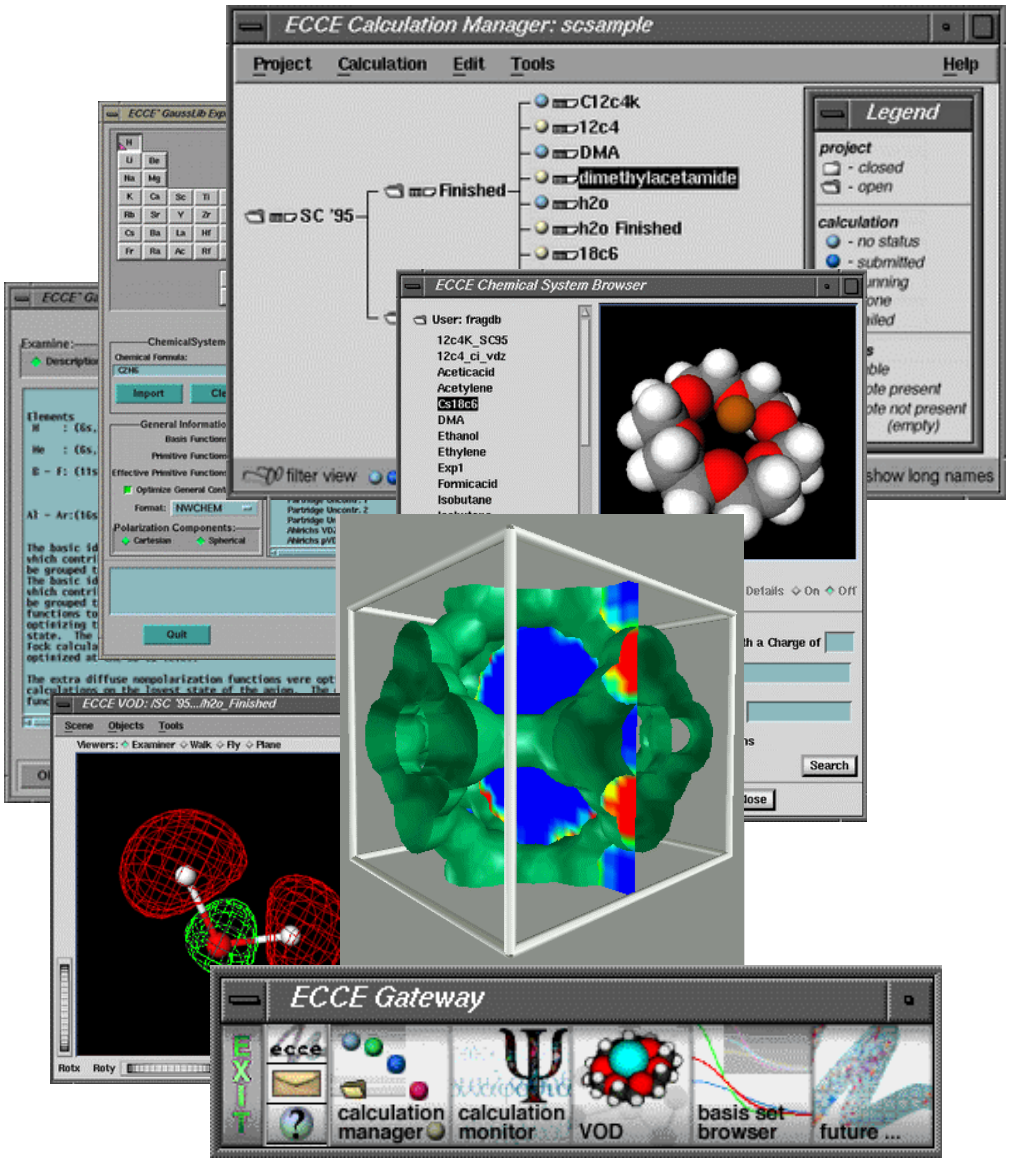
# Advancements
## What Have We Gained?

- **In 1992**
  - Model separations agents, *e.g.*, ether-alkali ions
- **In 2000**
  - *Serial computers*: prototype separation agents, *e.g.*, 18-crown-6
  - *Parallel computers*:* real-world separations agents, *e.g.*, Still's crown ether




* *With **NWChem** on 0.25-tf computer at PNNL.*

# Another Example
## Computational Chemical Environment




**ECCE**

extensible computational chemistry environment

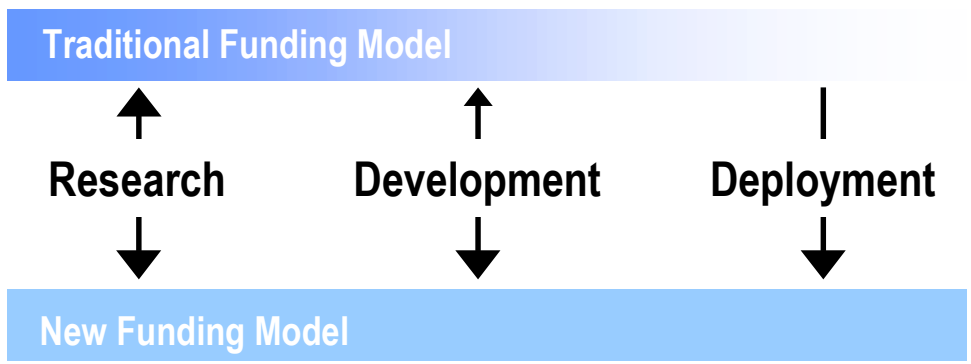
*An environment to assist the researcher in using NWChem*

## Key Features

- Point-and-click set up of calculations
- Browser-type management of both calculations and computers
- Chemistry-specific analysis and visualization tools
- Integrated data management

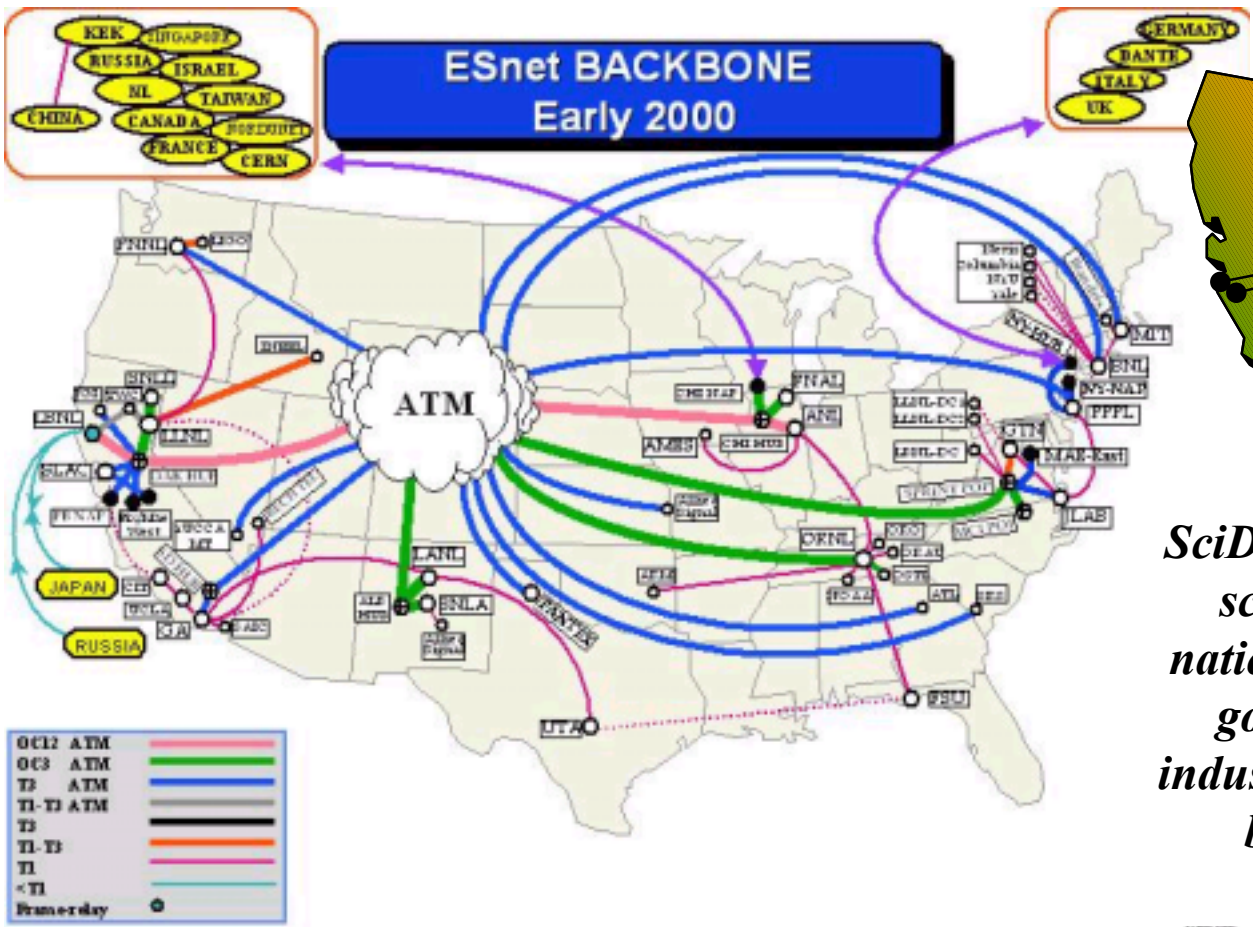
# SC Software Infrastructure
## Enabling Technology Centers

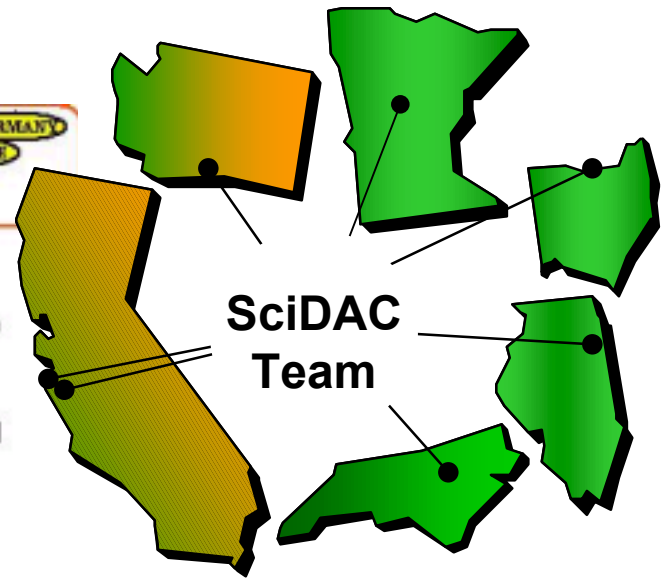
- **Teams of Mathematicians, Computer Scientists, Applications Scientists, and Software Engineers to ...**
  - Create mathematical and computing systems software to enable scientific simulation codes to take full advantage of the extraordinary capabilities of terascale computers
  - Work closely with Scientific Simulation Teams to ensure that the most critical computer science and applied mathematics issues are addressed in a timely fashion
  - Support the full software life cycle



# SC Software Infrastructure
## Collaboratories and Networks

**Create collaboratories, software, and networks to link geographically distributed researchers, data, and tools and to enable remote access to experimental and computational facilities.**




*SciDAC teams will be composed of scientists and engineers from national laboratories, universities, government laboratories, and industry and will be fully supported by electronic collaboration technology.*

# SC Software Infrastructure Plan

- **Initiate software development efforts in FY2001**
  - **Scientific Simulation Codes**: Competitively select 4-6 teams to begin development of advanced computational modeling and simulation codes ($20.0 million = BES: $2 million; BER: $8 million; FES: $3 million; HENP: $7 million)
  - **Enabling Technologies:** Competitively select 4-6 teams to begin development of mathematical and computing systems software and fund joint efforts ($27.0 million*)
  - **Collaboratories:** Competitively select 3-4 teams to continue development of collaboratory software ($10.1 million*)
- **Strengthen and broaden the software development efforts in FY2002 and beyond (*new funds required*)**

* *OASCR total reduced by approx. $10 million for Laboratory Technology Research program.*

# Scientific Computing Hardware Infrastructure

# SC Hardware Infrastructure
## Robust, Agile, Effective & Efficient

- **Flagship Computing Facility**
  - To provide robust, high-end computing resources for *all* SC research programs
- **Topical Computing Facilities**
  - To provide the most effective and efficient computing resources for a set of scientific applications
  - To serve as a focal point for a scientific research community as it adapts to new computing technologies
- **Experimental Computing Facilities**
  - To assess new computing technologies for scientific applications

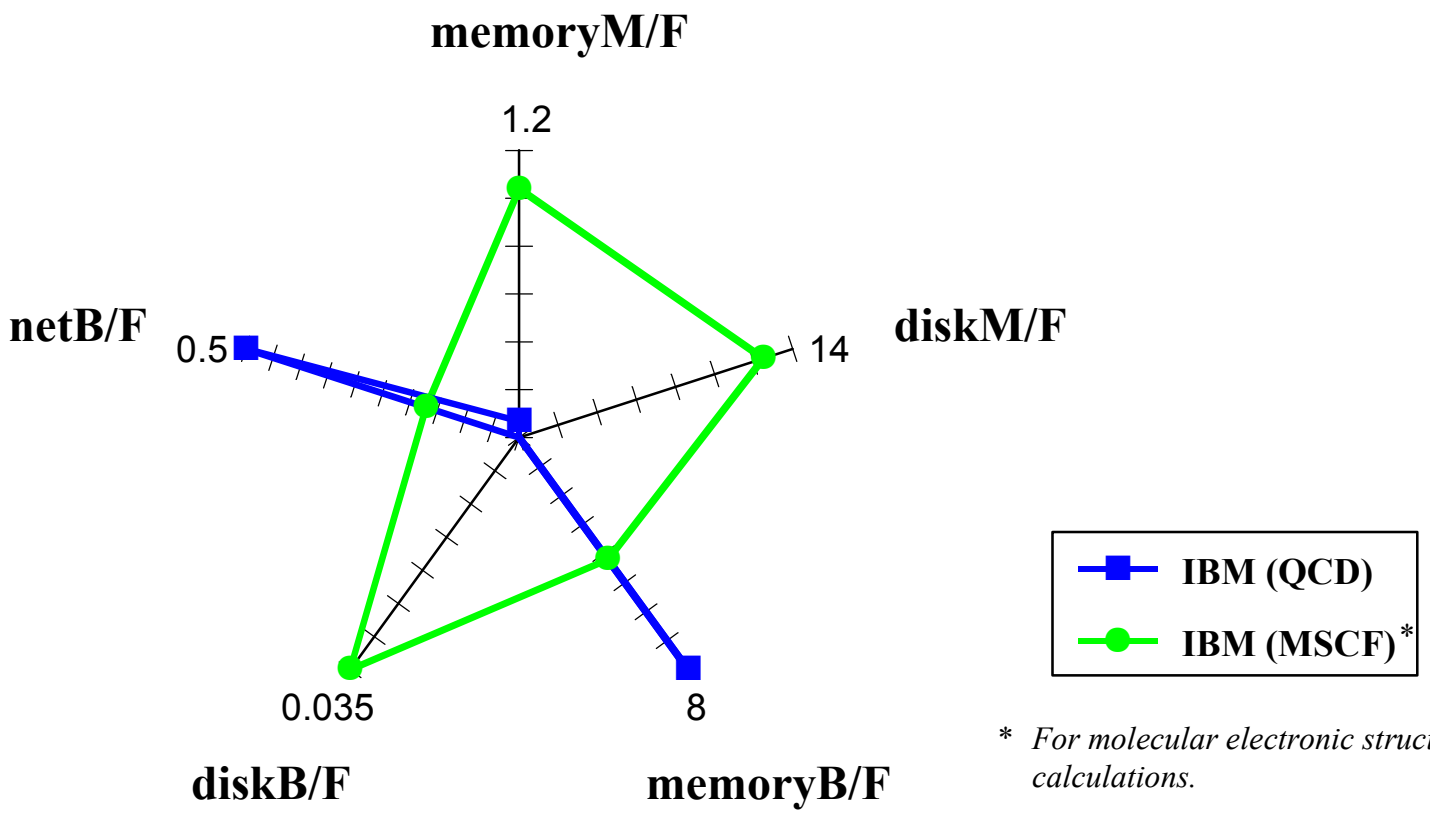
# Why Topical Facilities?
## Variation in Scientific Application Needs*

| Code | Application | Time (TFLOPS-HRS) | Memory (TBYTES) | Storage (TBYTES) | Node I/O (MBYTES/S) |
|---|---|---|---|---|---|
| **Cactus** | Astrophysics | 300 | 1.8 | 20 | 5 |
| **ARPS** | Weather | 25 | 0.25 | 16 | 18 |
| **MILC** | Particle Physics | 10,000 | 0.2 | 1 | 3 |
| **PPM** | Turbulent Flow | 500 | 0.5 | 54 | 6 |
| **PUPI** | Liquids | 150 | 0.1 | 0.2 | 3 |
| **ASPCG** | Fluid Dynamics | 5,000 | 0.5 | 50 | 3 |
| **ENZO** | Galaxies | 1,000 | 0.9 | 10 | 12 |
| | **Variation** | **400x** | **18x** | **100x** | **6x** |

* *From "High-level Application Resource Characterization," NSF/PACI National Computational Science Alliance, May 2000. Reported by permission of Dr. D. A. Reed, Director, National Center for Supercomputing Applications.*

# Topical Computing Facilities

## Computer Specifications: QCD & Chemistry




* *For molecular electronic structure calculations.*

# Why Topical Facilities?
## A Response to the Software Challenge

- **To provide the organizational framework needed for multidisciplinary activities**
  - Addressing software challenges require strong, long term collaborations among disciplinary computational scientists, computer scientists, and applied mathematicians
- **To provide the organizational framework needed for the development of community codes**
  - Implementation of many scientific codes requires a wide range of disciplinary expertise
- **Organizational needs will continue as computers advance to petaflops scale**

# Topical Computing Facilities

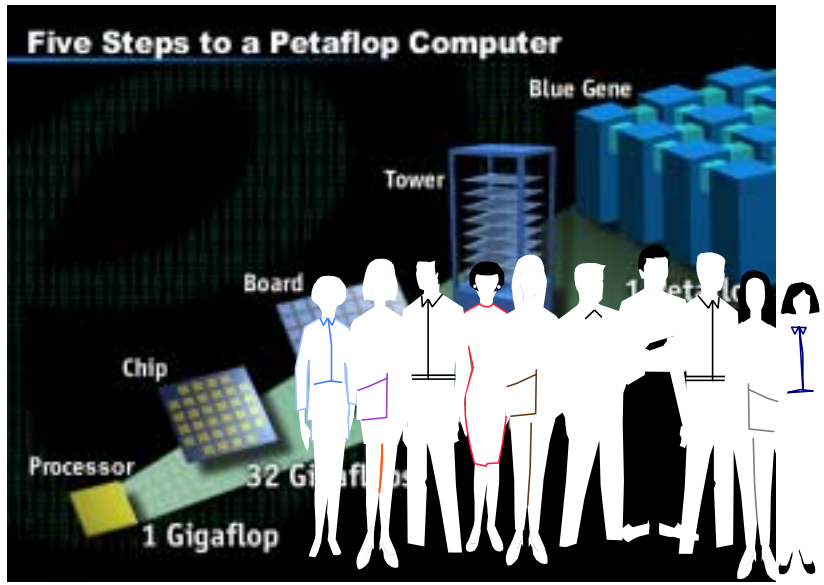
## Selection Criteria

- **Importance of the scientific application** to the mission of the U.S. Department of Energy
- **Need for extraordinary computing resources** to address problems of critical scientific and national importance, **ability to fully use** these resources
- **Ability to advance the state-of-the-art** in computational modeling and simulation in the selected application area
- **Ability to provide cost efficiencies or capability enhancements** over and above that achieved in Flagship Facility

# Why Experimental Facilities?

- **Need an organized approach for evaluation of new computing technologies (processors, switches, *etc*.)**
  - Although we are currently on a plateau vis-à-vis computer architectures, this will not last through the end of the decade
  - Examples of new approaches include PIM (processors-in-memory), HTMT (hybrid technology-multithread technology)
- **Need an organized approach for interacting with computer designers as early as possible**
  - Computer designers have many variables to consider – some beneficial for scientific computing, others not
  - Earlier the scientific community can provide input, the more likely the advice will be heeded

# Elements of Experimental Computing Facility



**Technologies Evaluation Teams**

**Core Teams + Distributed Team Members**

**Code Development Teams**

**@ Flagship Computing Facility**

**@ Topical Computing Facilities**

# SC Hardware Infrastructure Plan

- **Upgrade existing Flagship Facility in FY2001**
  - NERSC-3 to 5-teraflops ($5.8 million*)
  - ESnet ($3.5 million*) + Network Testbed ($1.0 million*)
- **Upgrade Advanced Computing Research Facilities in FY2001 ($2.0 million*)**
- **Add new facilities in FY2002 and beyond**
  - Competitively establish a number of Topical Computing Facilities, beginning in FY2002 (*new funds required*)
  - Establish up to two (2) Experimental Computing Facilities, beginning in FY2002 by recompeting the Advanced Computing Research Facilities (*no new funds required*)

* *OASCR total reduced by approx. $10 million for Laboratory Technology Research program.*

# Elements of Topical Computing Facility

## Computing Systems

## Code Development Teams

**Core Teams + Distributed Team Members**

## Scientific Application Users

# Proposed FY2001 Investments

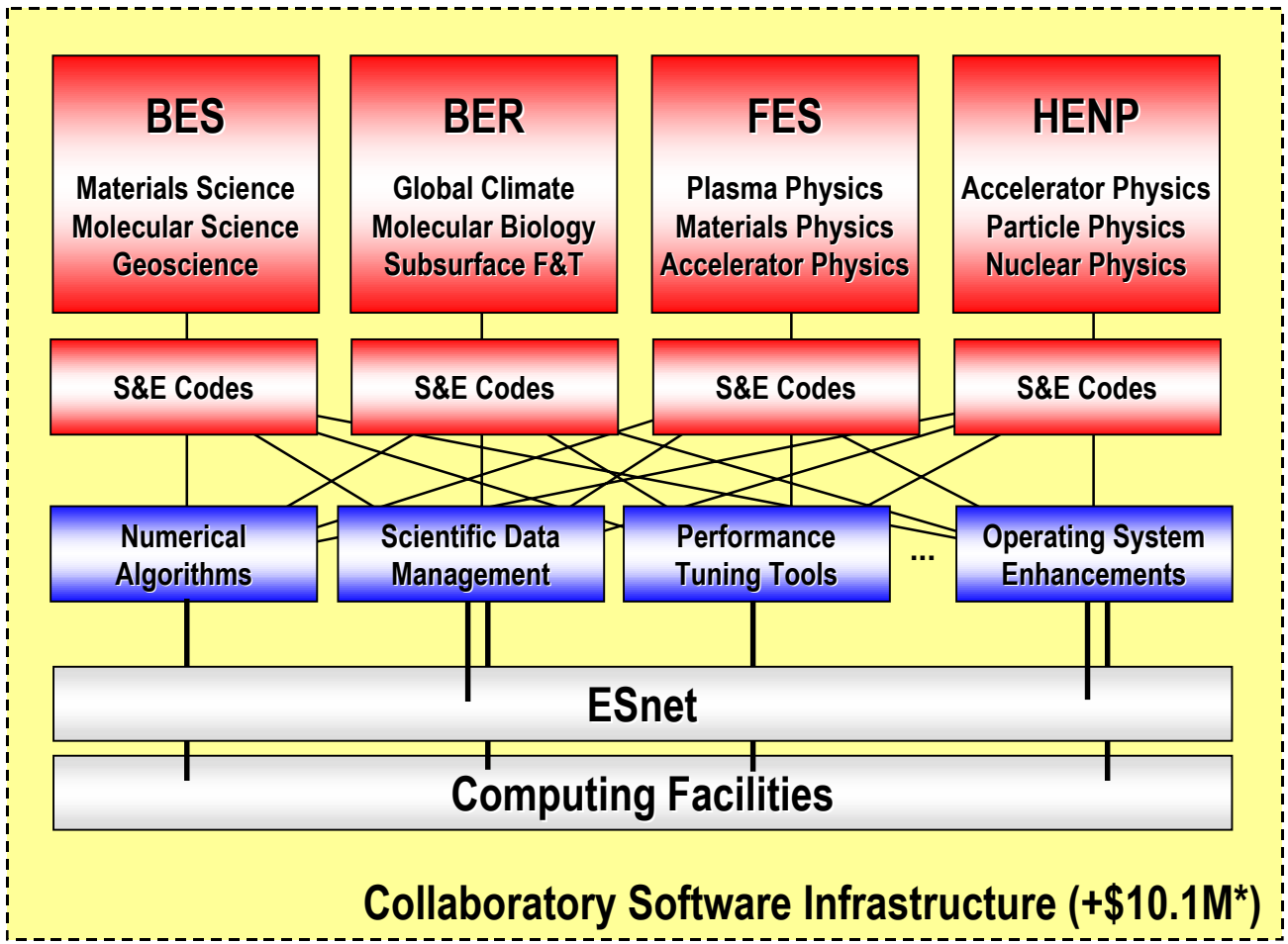
## Scientific Discovery through Advanced Computing

*Investments in computational modeling and simulation in the Office of Science are driven by scientific problems derived from DOE's missions.*

**Scientific Code Development Teams (+$20.0M)**

**Enabling Technology Centers (+$27.0M*)**

**Computing Hardware Infrastructure (+$12.3M*)**

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