Bringing the Grid to Chemical Engineering

- Opening Talk at the 1998 Foundations of Computer Aided Process Operations Conference in Snowbird, Utah
- July 5, 1998

Bringing the Grid to Chemical Engineering

Larry Smarr

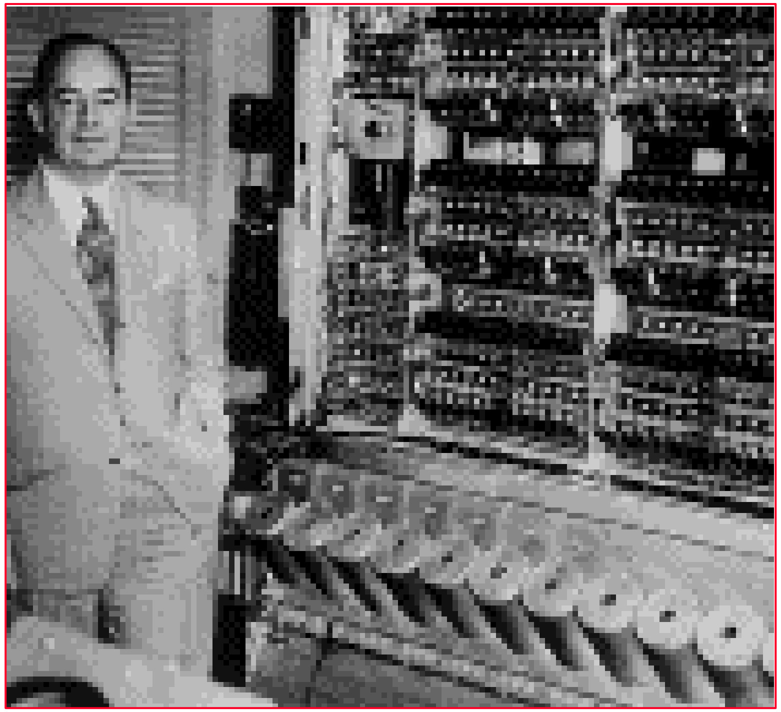
Director

National Center for Supercomputing Applications

National Computational Science Alliance

University of Illinois at Urbana-Champaign

A Chemical Engineer Started Modern Digital Computing!



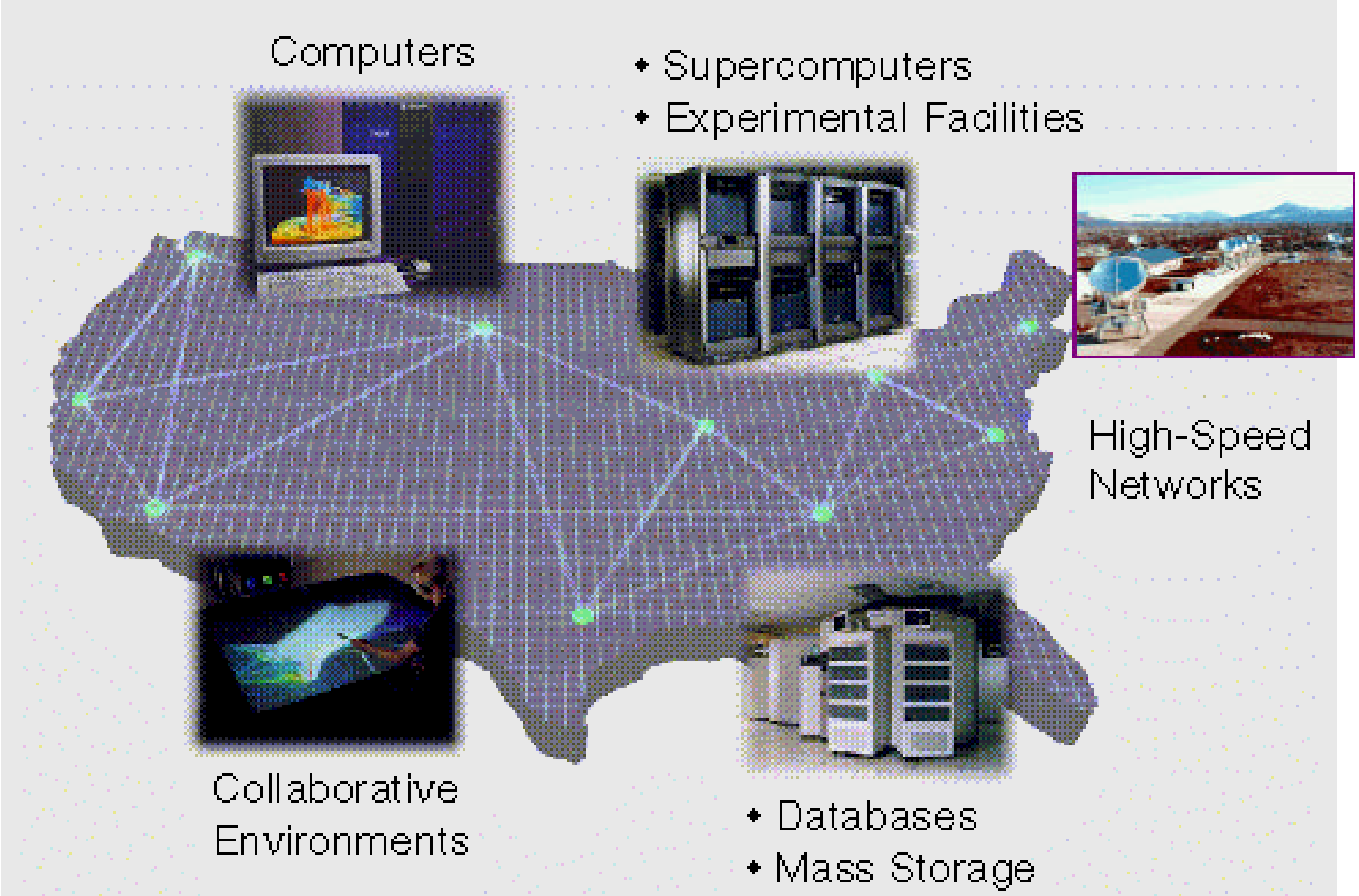
John von Neumann

B.S. Chemical Engineering
ETH Zurich

Outline of Presentation

- Introducing the Grid
- New Directions in Computing
- Challenges to the Chemical Industry
- The Chemical Engineer's Workbench
- The Killer App for the Grid: Tele-Immersion
- Conclusions

The Grid Links People with Distributed Resources on a National Scale



The Emerging Concept of a National Scale Information Power Grid

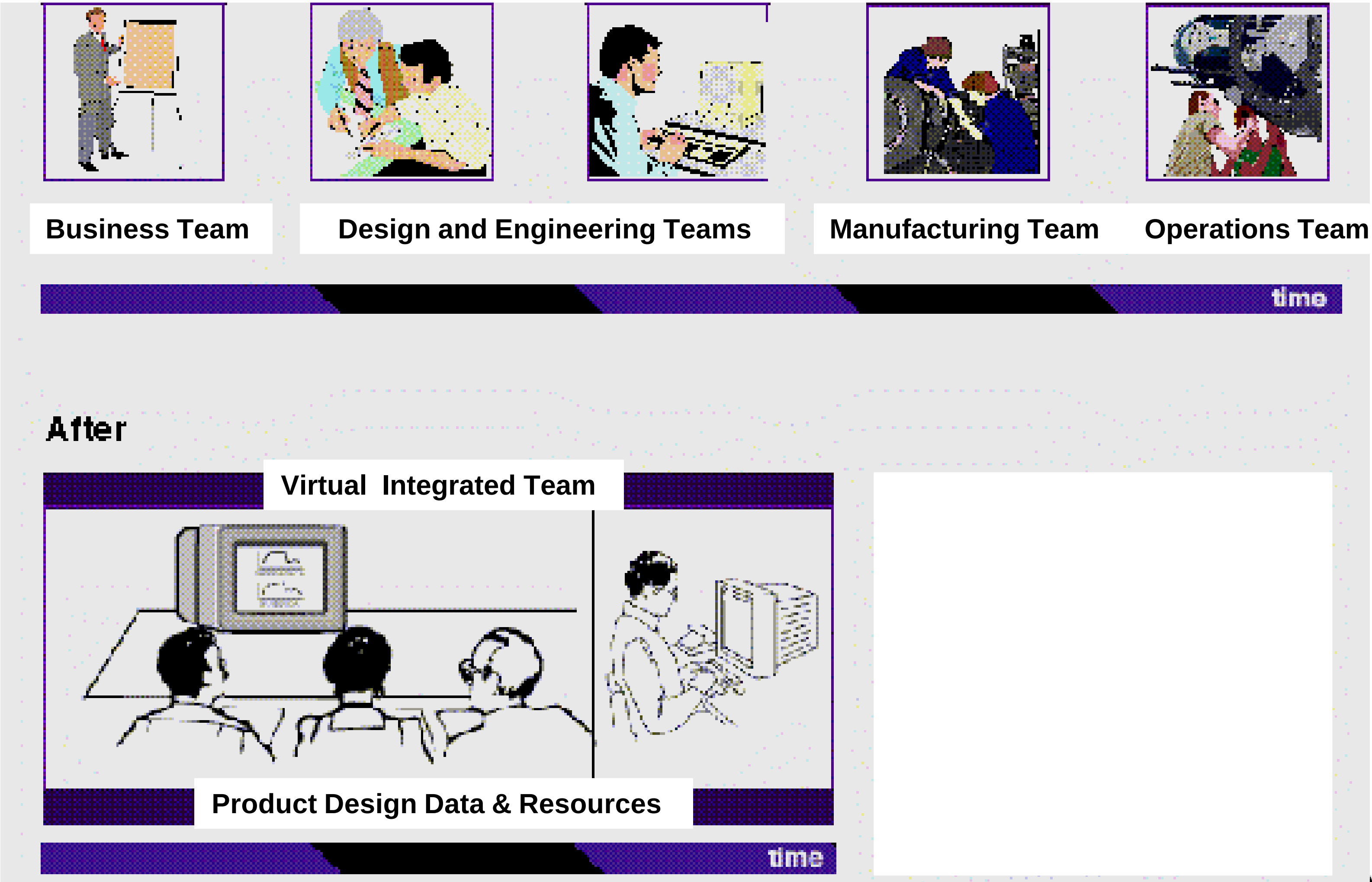
Imagine a national computing and information infrastructure that allowed everyone to access the information resources of the nation in much the same way that one accesses electrical power today; an "Information Power Grid"

Your Electrical Power Available Here

Your Information Power Available Here

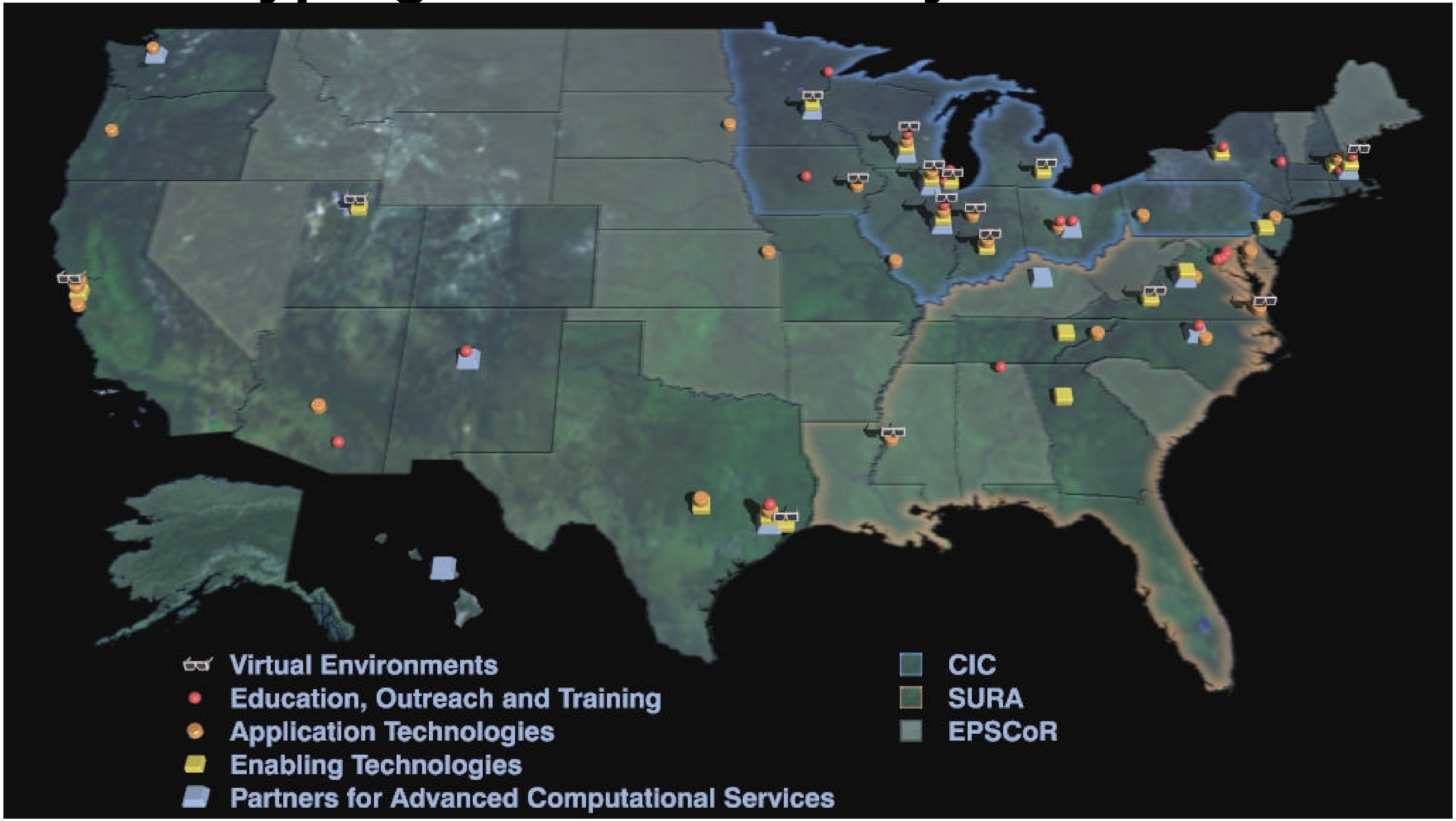
The Grid Can Unify Enterprise Business Processes

Before



http://science.nas.nasa.gov/Groups/Tools/IPG

The Alliance National Technology Grid - Prototyping the 21st Century Infrastructure

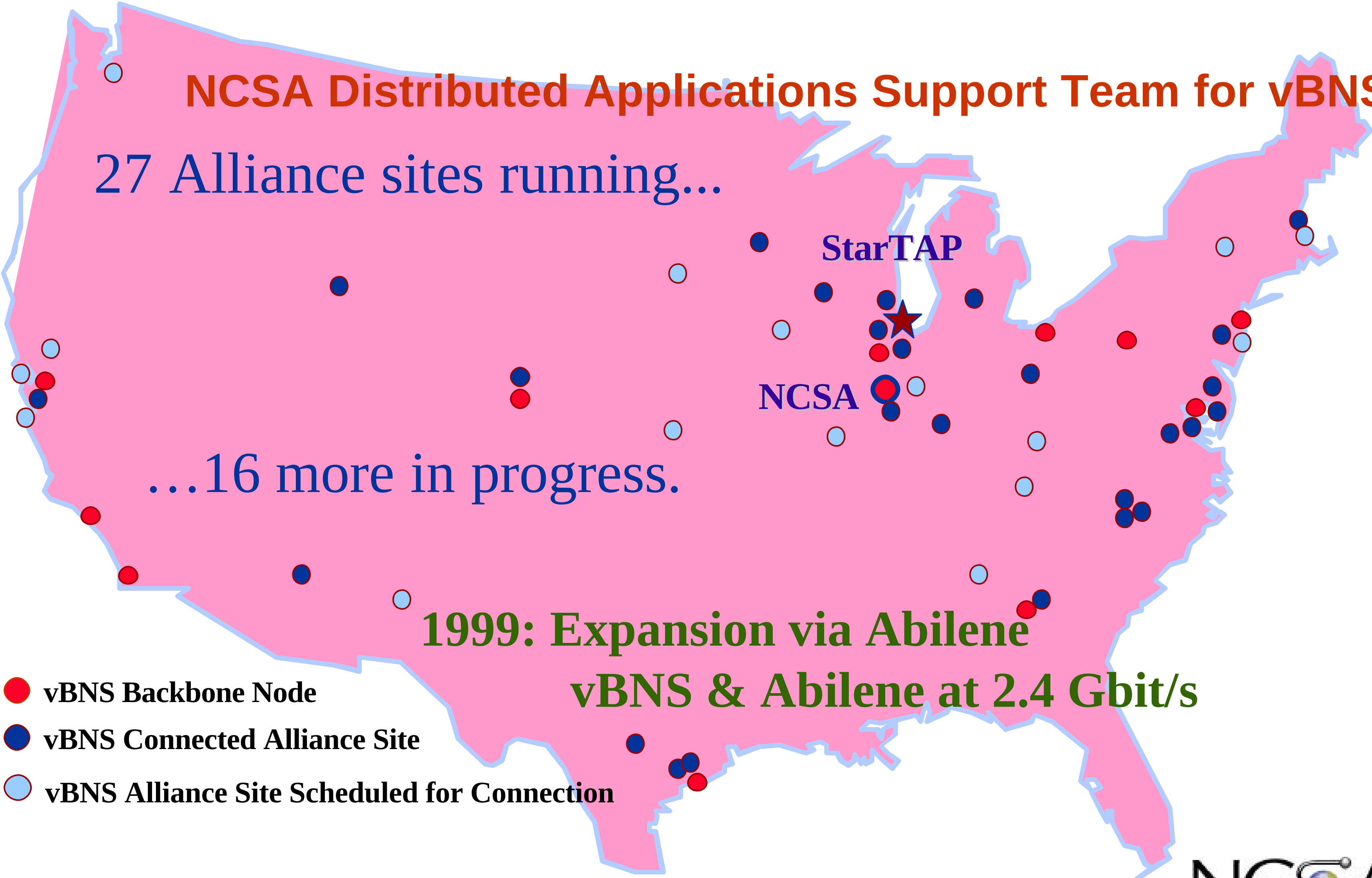


FY98 Assembling the Links in the Grid with NSF's vBNS Connections Program

NCSA Distributed Applications Support Team for vBNS

27 Alliance sites running...

…16 more in progress.



1999: Expansion via Abilene

vBNS & Abilene at 2.4 Gbit/s

Source: Charlie Catlett, Randy Butler, NCSA

NCSA National Computational Science Alliance

How Applications Teams Drive the Alliance

- **Cosmology**
  - **Metacomputing**
- **Environmental Hydrology**
  - **Immersive Collaboration**
- **Chemical Engineering**
  - **Virtual Prototyping**
- **Bioinformatics**
  - **Distributed Data**
- **Nanomaterials**
  - **Remote Microengineering**
- **Scientific Instruments**
  - **Virtual Observatories**

- Multidiscipline Domains
- Multiscale Interactions
- Complex Geometries
- Full-up Virtual Prototyping
- Large Scale Optimization

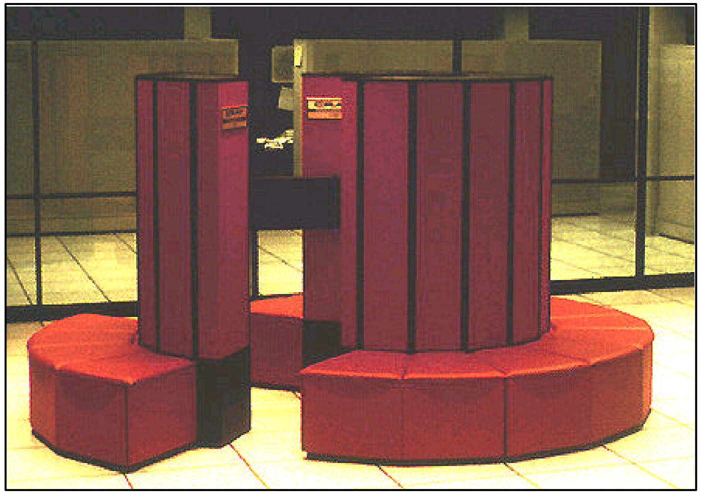
NCSA Industrial Partners Drive Innovation

- Allstate Insurance Co.
- Boeing Company
- Caterpillar Inc.
- Eastman Kodak Co.
- FMC Corporation
- Ford Motor Company
- J. P. Morgan
- Motorola, Inc.
- Phillips Petroleum Co.
- SABRE Group, Inc.
- Schlumberger
- Sears, Roebuck & Co.
- Shell Oil Company

Enterprise Management-
Convergence of Commercial and Technical Computing

- **The Web Browser as a Universal Interface**
  - To Data, Video, Instruments, Computing
- **Virtual Teams In Business and Research**
  - Intranets and Collaborative Environments
- **Emergence of Distributed Object Architecture**
  - Java, ActiveX, CORBA, Integrated Thru the Web
- **From Scientific Visualization to Info. Viz.**
  - Data Mining Petabyte Archives
- **Microprocessor Market Convergence**
  - NT/Intel Challenging UNIX/RISC

The Continuing Exponential Agent of Change



1985 Cray X-MP

Cost: $8,000,000

60,000 watts of power

No Built in Graphics

56 kbps NSFnet Backbone

1997 Nintendo 64

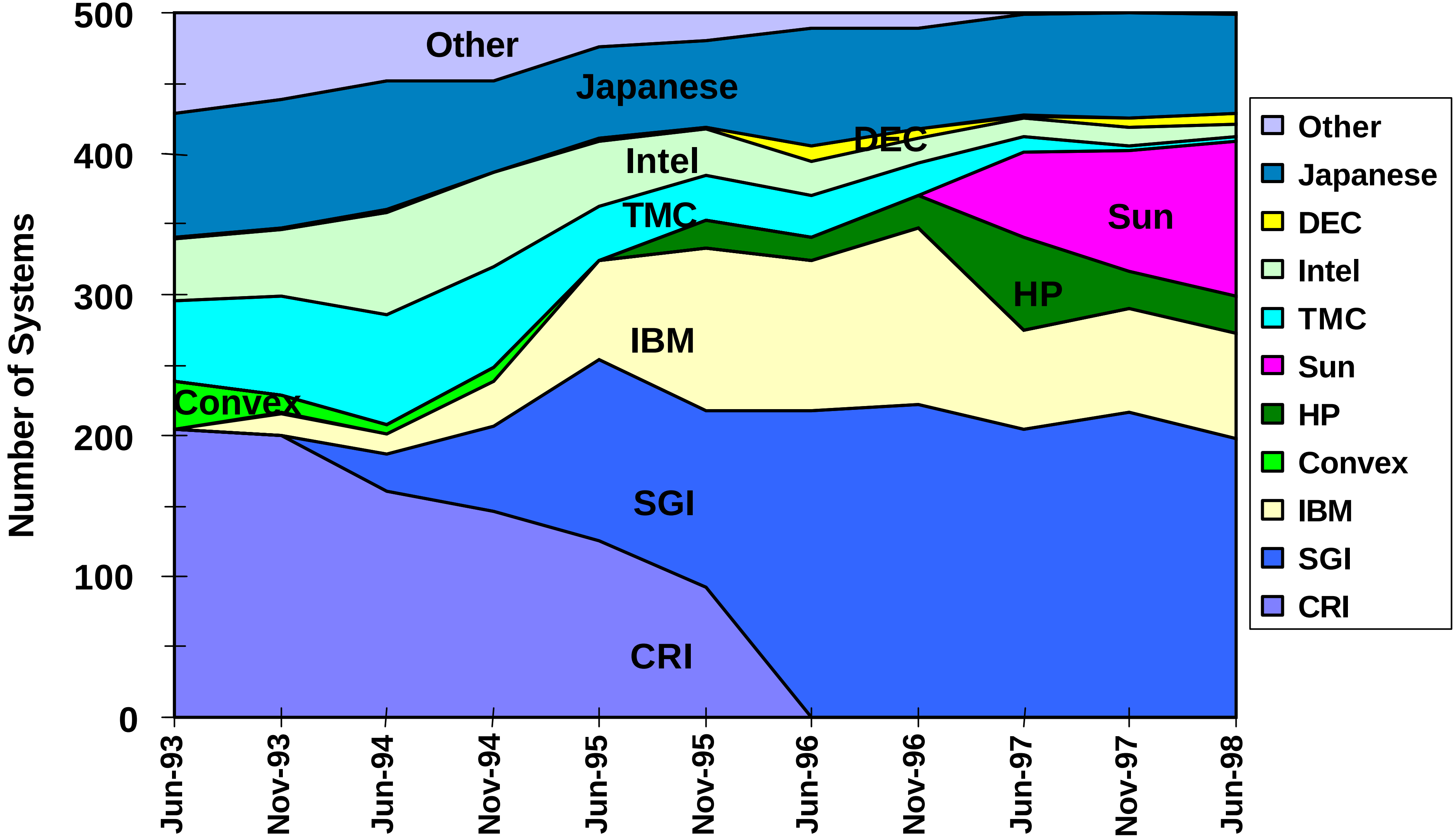
Cost: $149

5 watts of power

Interactive 3D Graphics

64 kbps ISDN to Home

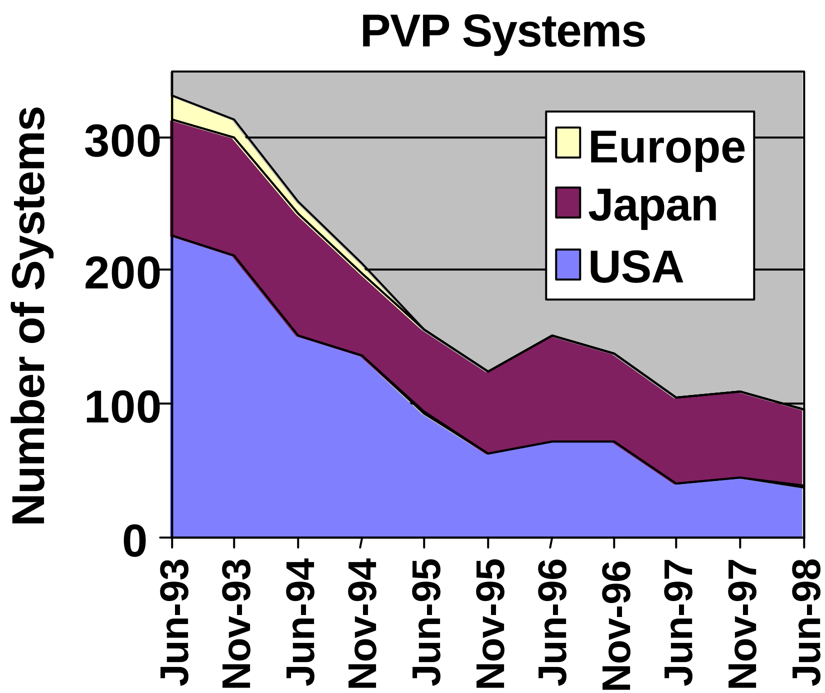
TOP500 Systems by Vendor - A Market Revolution

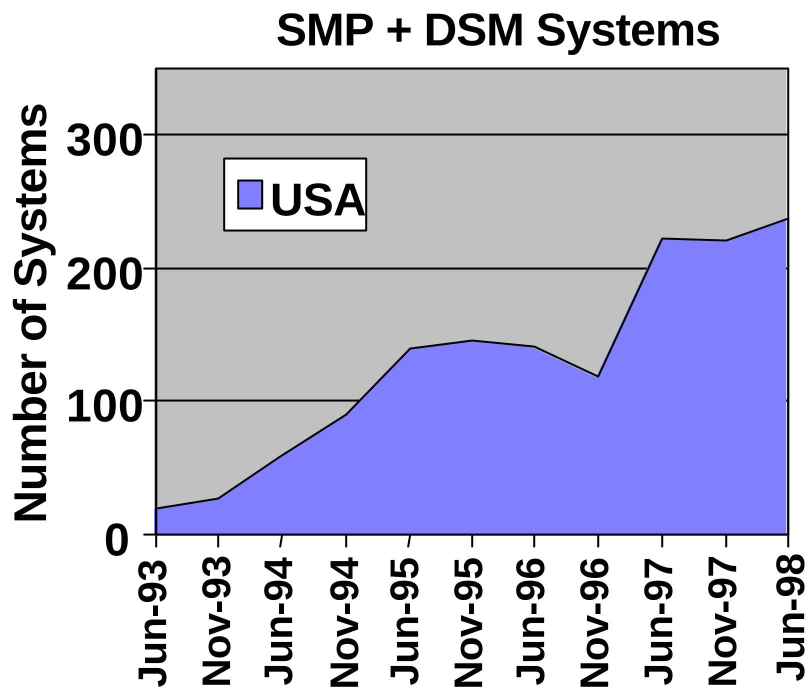


TOP500 Reports: http://www.netlib.org/benchmark/top500.html

National Computational Science Alliance

Shared Memory Microprocessors Replacing Vector Systems in Top 500

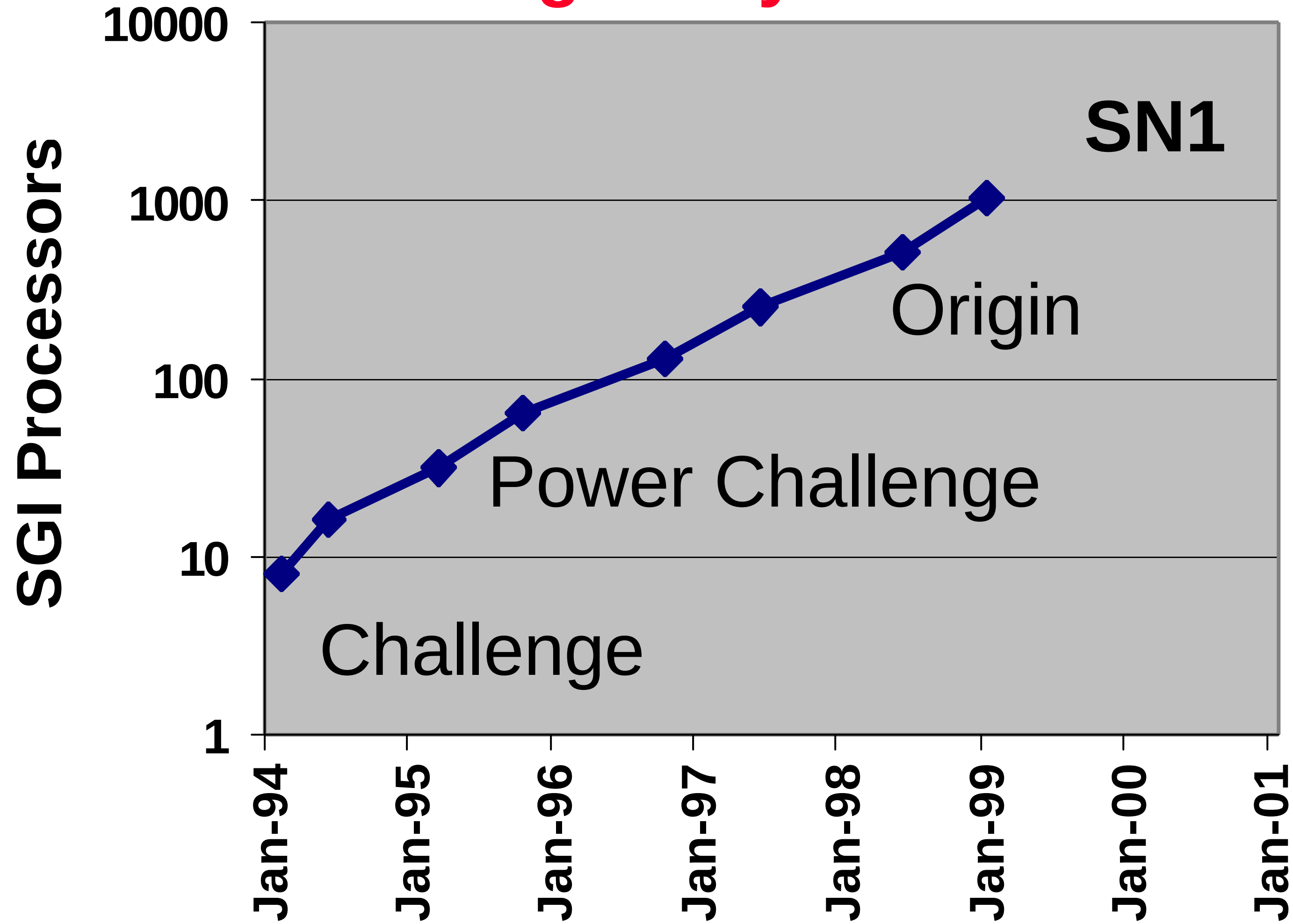




Vector Processors **Microprocessors**

NCSA is Combining Shared Memory Programming with Massive Parallelism

Doubling Every Nine Months!

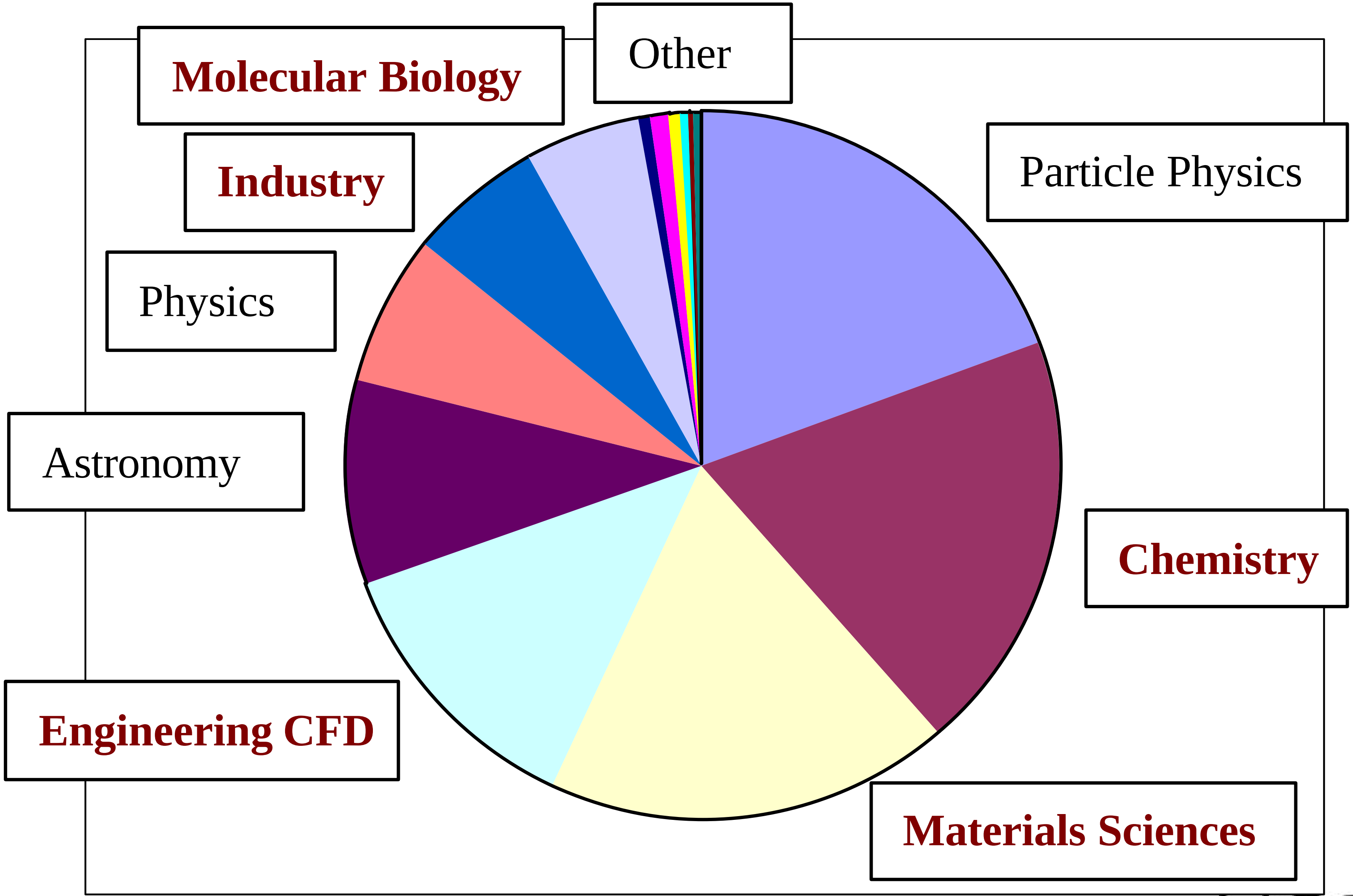


High-End Architecture 2000-
Scalable Clusters of Shared Memory Modules

Each is 4 Teraflops Peak

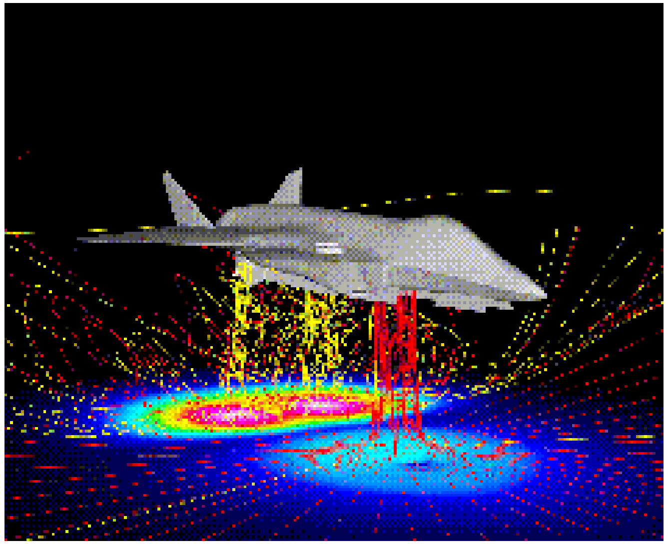
- NEC SX-5
  - 32 x 16 vector processor SMP
  - 512 Processors
  - 8 Gigaflop Peak Vector Processor
- IBM SP
  - 256 x 16 RISC Processor SMP
  - 4096 Processors
  - 1 Gigaflop Peak RISC Processor
- SGI Origin Follow-on - SN1
  - 8 x 256 RISC Processor DSM
  - 2048 Processors
  - 2 Gigaflop Peak EPIC Processor

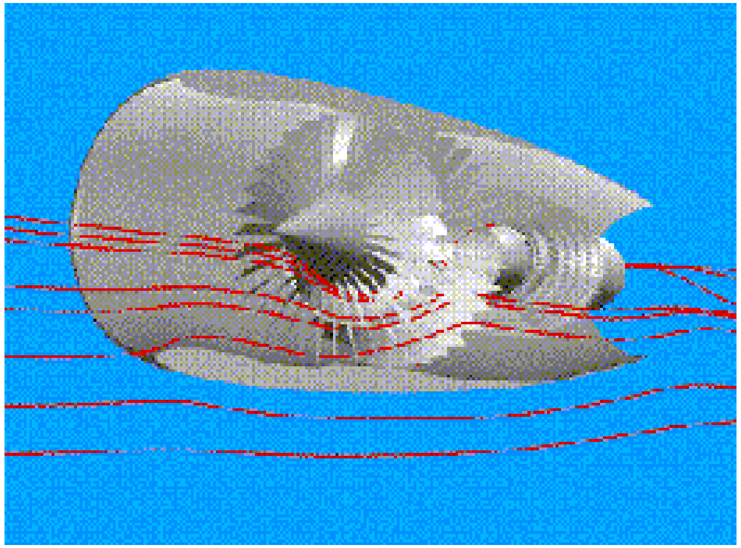
Disciplines Using the NCSA Origin 2000 CPU-Hours in March 1998



NASA Computational Aerosciences

- First-of-a-kind aerodynamic sim. of adv. ASTOVL in near-hover ground effect with strong fountain



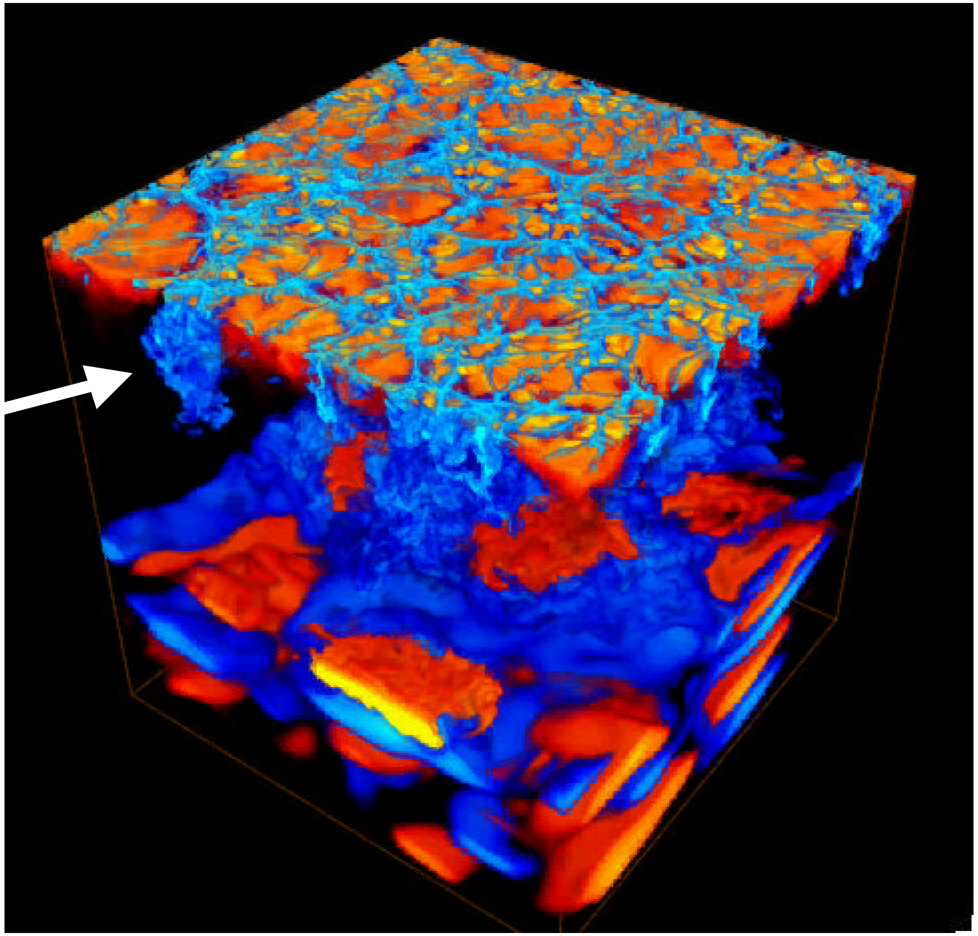


- 8X speedup on compressor analysis code, 5X for combustion flow solver
- Design time reduced from 18 to 14 months by 9/97
- $3.33 million saved per design

http://science.nas.nasa.gov/Groups/Tools/IPG

Simulation of Convective Mixing

Constant Temperature on Top

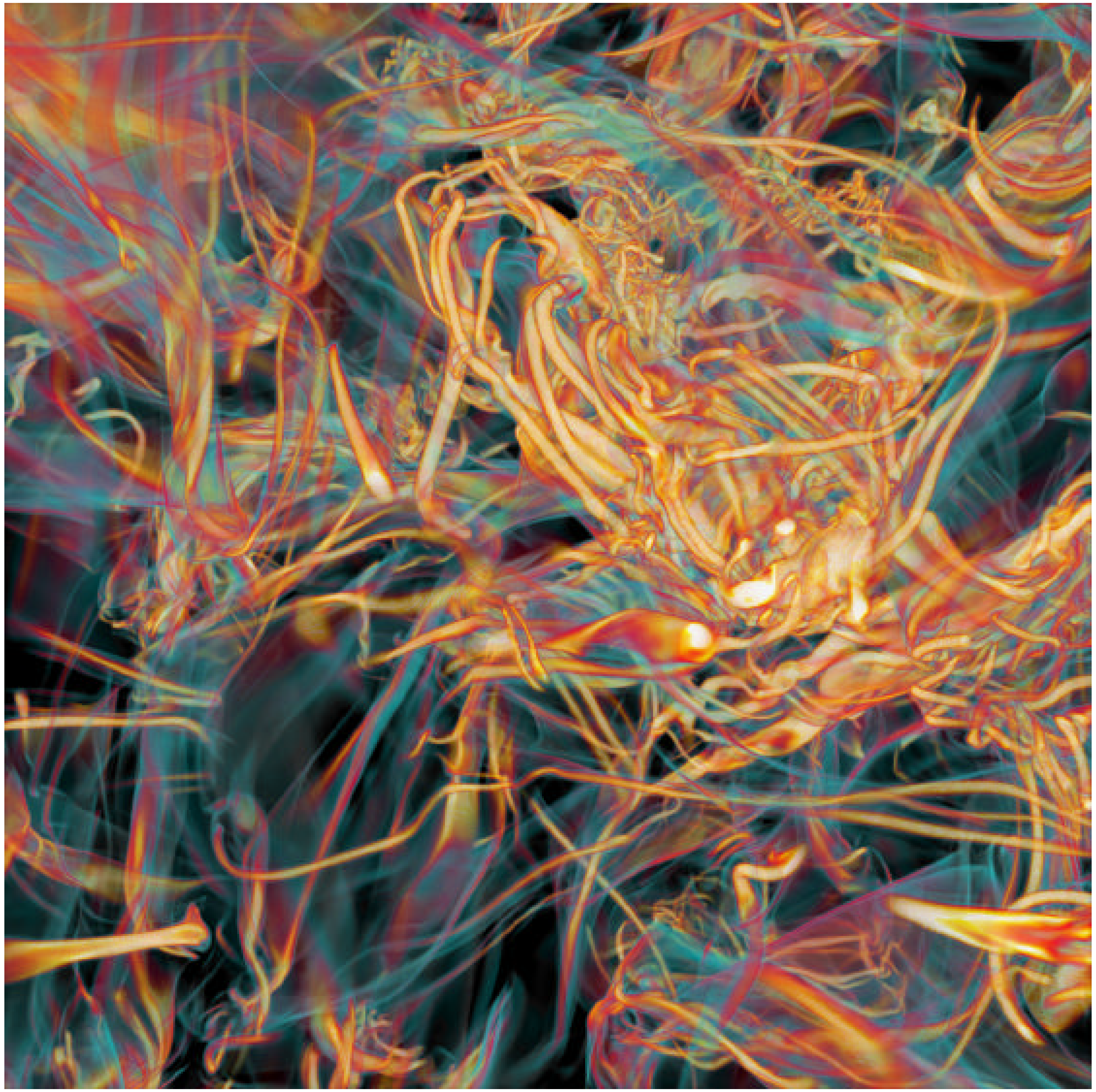


Cooler Descending Plume

Constant Heat Flux on Bottom

- 512x512x512 Grid
- 285,000 CPU-Hours on PSC T3D
- Bottom Half Stable, Top Half Unstable (Thermal Diffusivity Varies with Height)
- Color Shows Temperature Fluctuations (Red Hot, Blue Cool)

High-End Computing Enables High Resolution of Flow Details



1024x1024x1024-
A **Billion** Zone
Computation of
Compressible
Turbulence

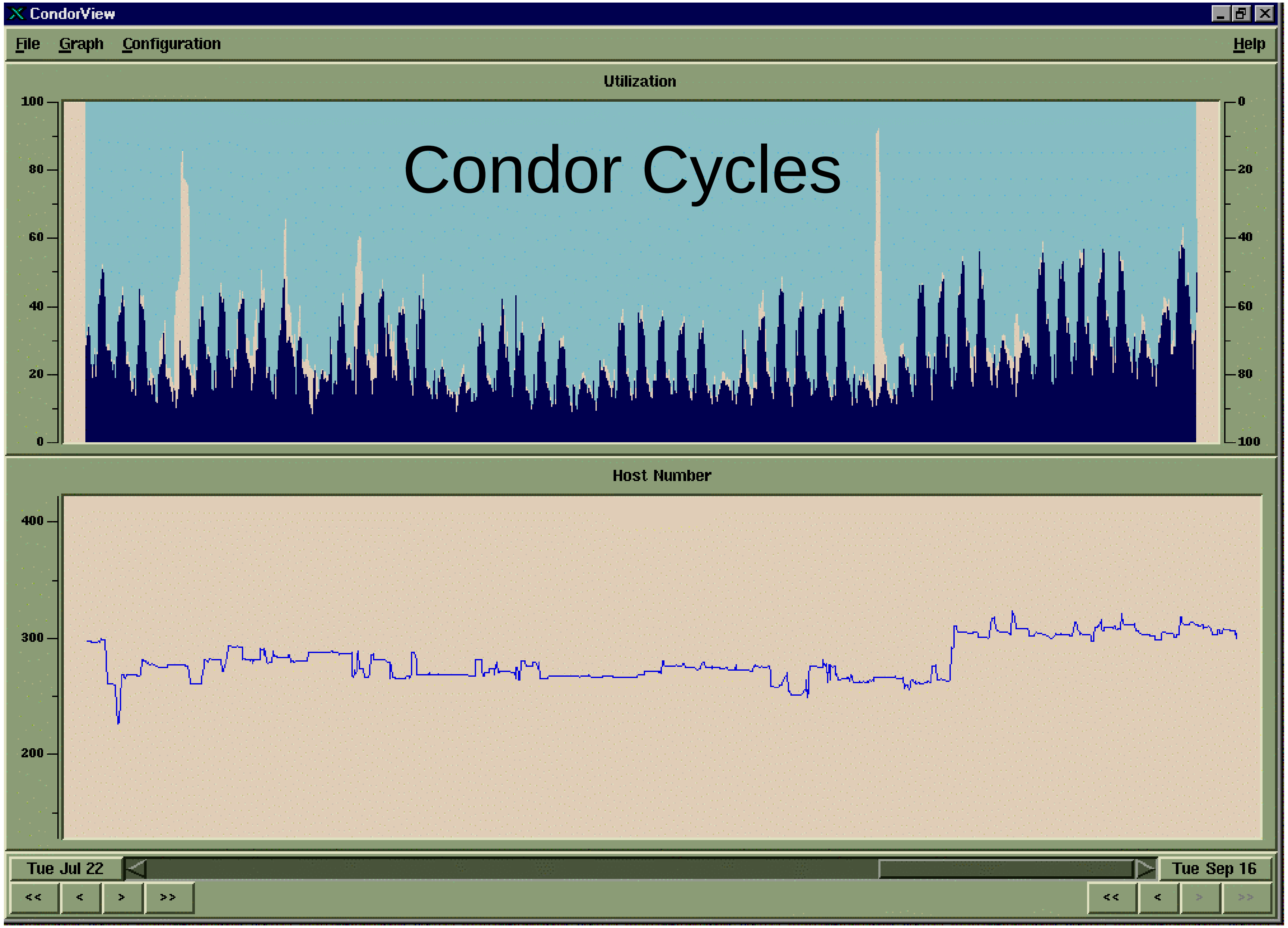
This Simulation Run
on Los Alamos SGI
Origin Array

U. Minn.SGI Visual
Supercomputer
Renders Images

Vorticity

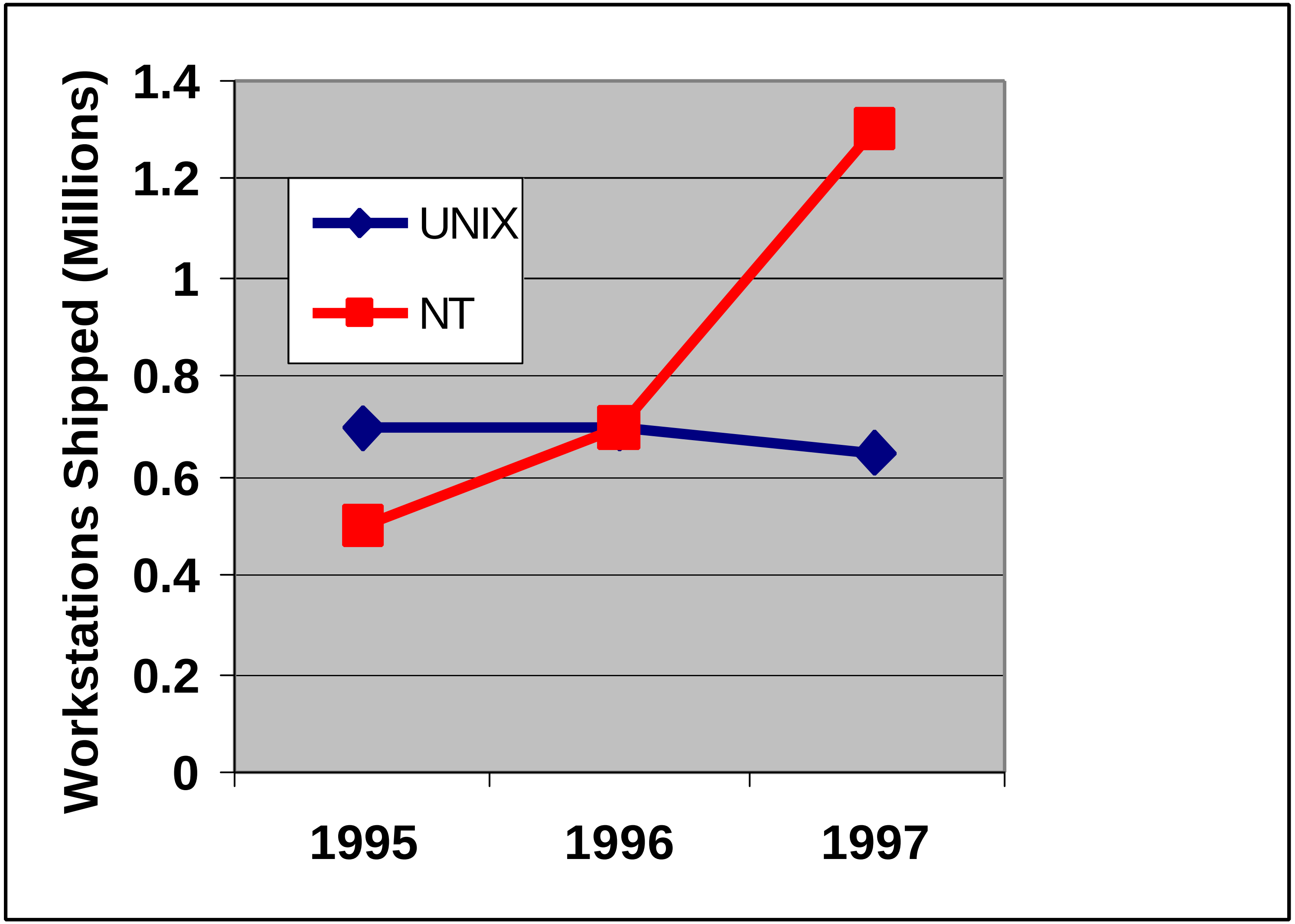
LCSE, Univ of Minnesota www.lcse.umn.edu/research/lanlrun/

Harnessing Distributed UNIX Workstations - University of Wisconsin Condor Pool



CondorView, Courtesy of Miron Livny, Todd Tannenbaum(UWisc)

NT Workstation Shipments Rapidly Surpassing UNIX

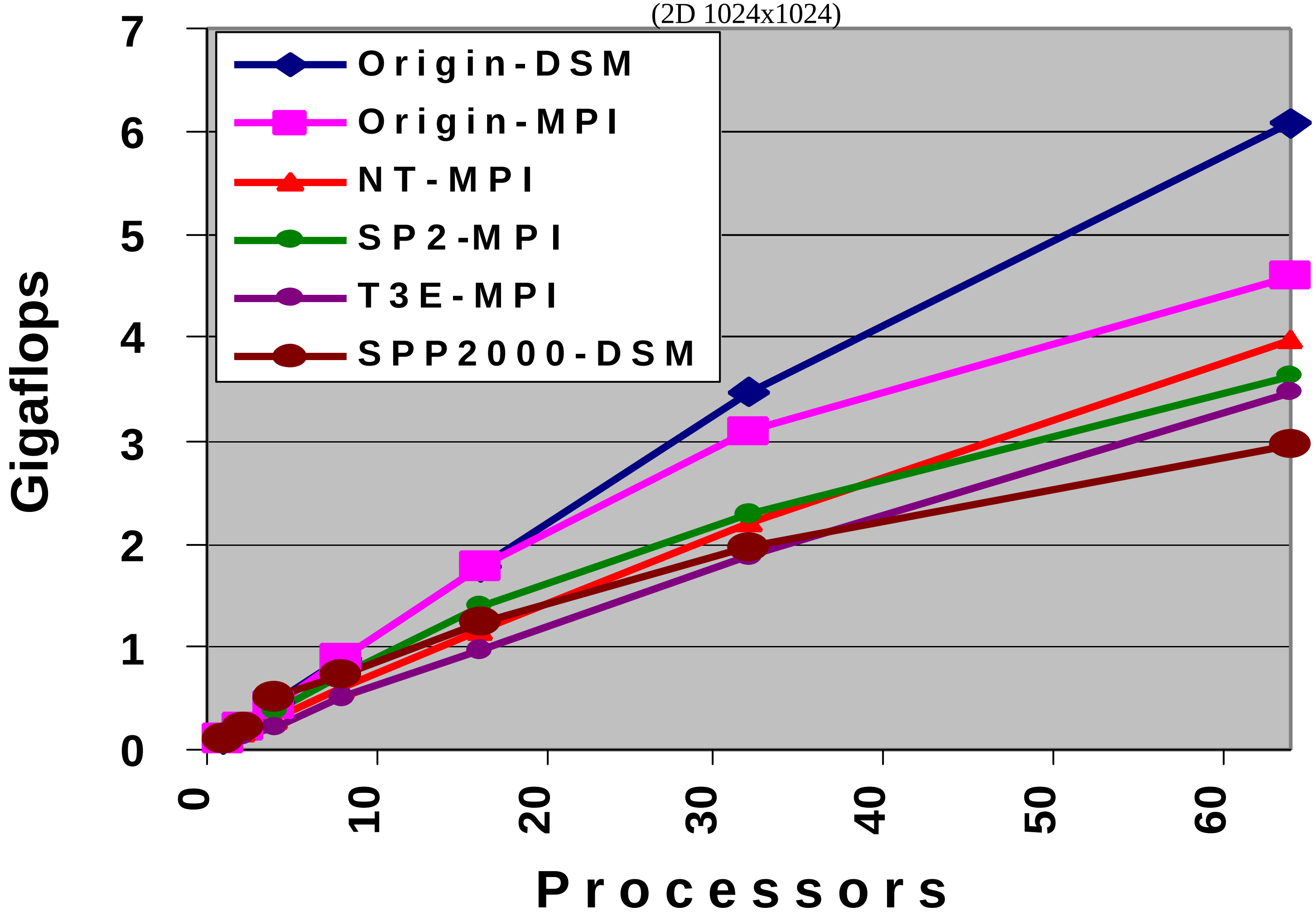


Source: IDC, Wall Street Journal, 3/6/98

Solving 2D Navier-Stokes Kernel - Performance of Scalable Systems

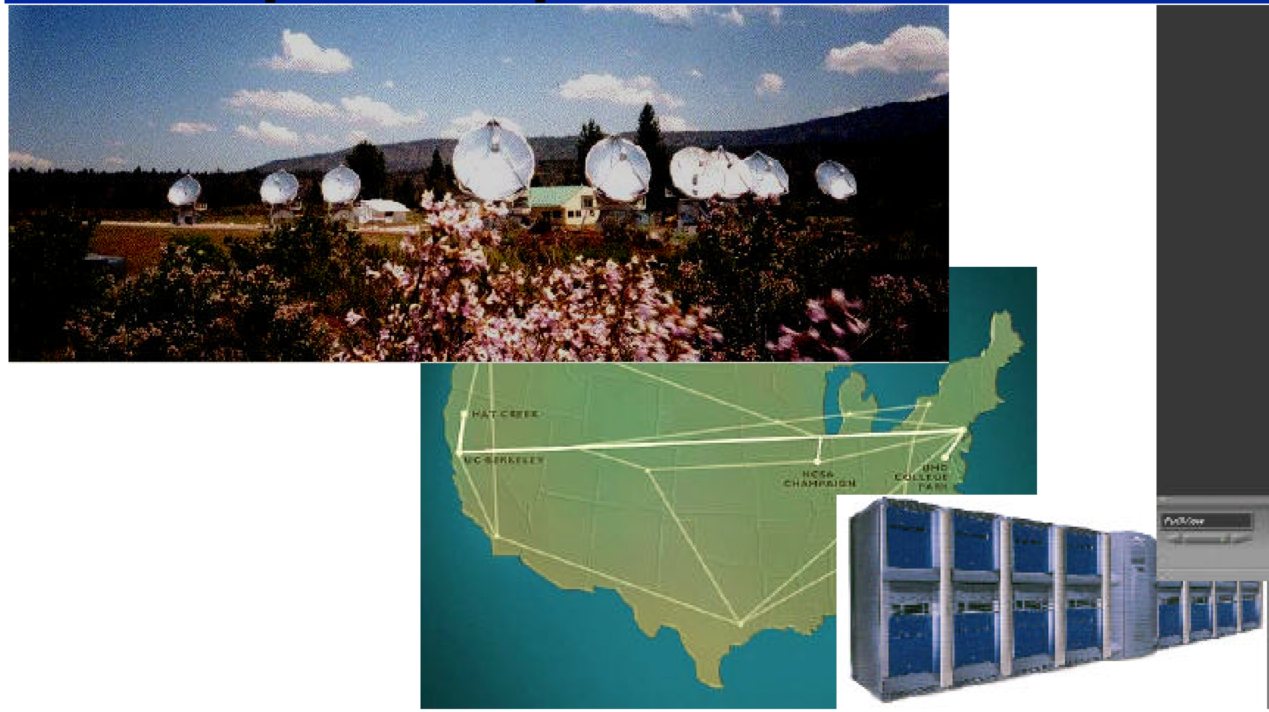
Preconditioned Conjugate Gradient Method With Multi-level Additive Schwarz Richardson Pre-conditioner

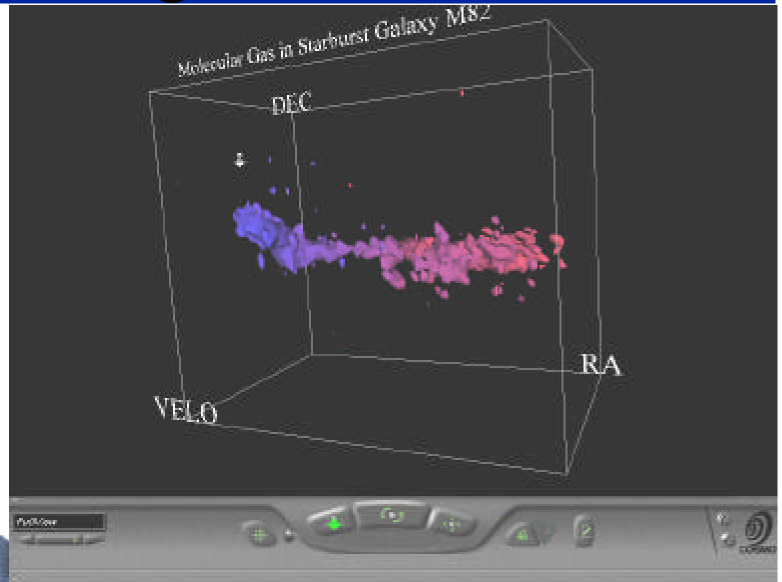
(2D 1024x1024)



Source: Danesh Tafti, NCSA

The Grid Links Remote Sensors With Supercomputers, Controls, & Digital Archives

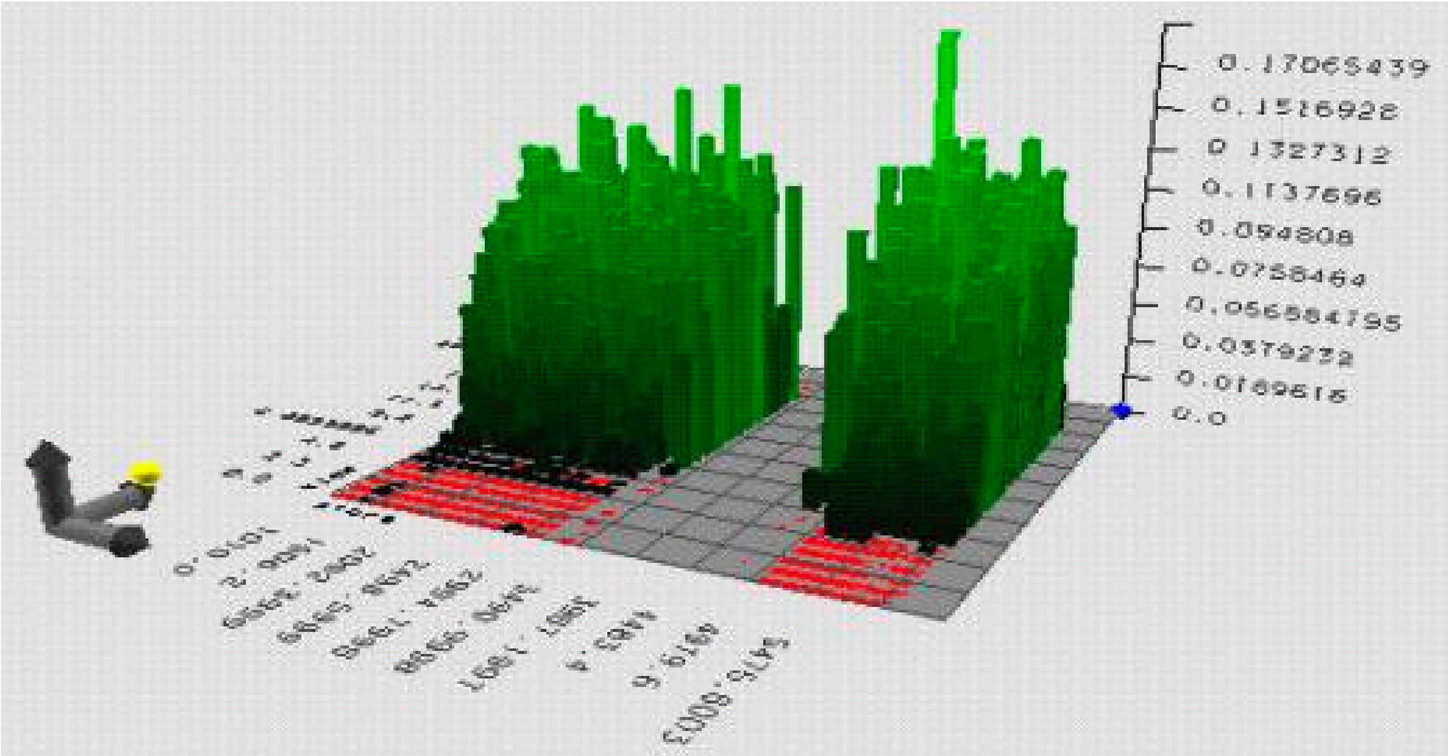




Starburst Galaxy M82

- **Alliance Scientific Instrument Team**
  - Radio Astronomy and Biomedicine
  - Collaborative Web Interface
  - Real Time Control and Steering

Sears Pioneers Massive Data Mining and Information Visualization at NCSA



- **1998 VLDB Survey Program Grand Prize Winner**
  - **Largest Database**
    - **4.7 Terabytes of Data**
  - **10 Terabyte Total Disk Space Capacity**
    - **Storage Provided by EMC**

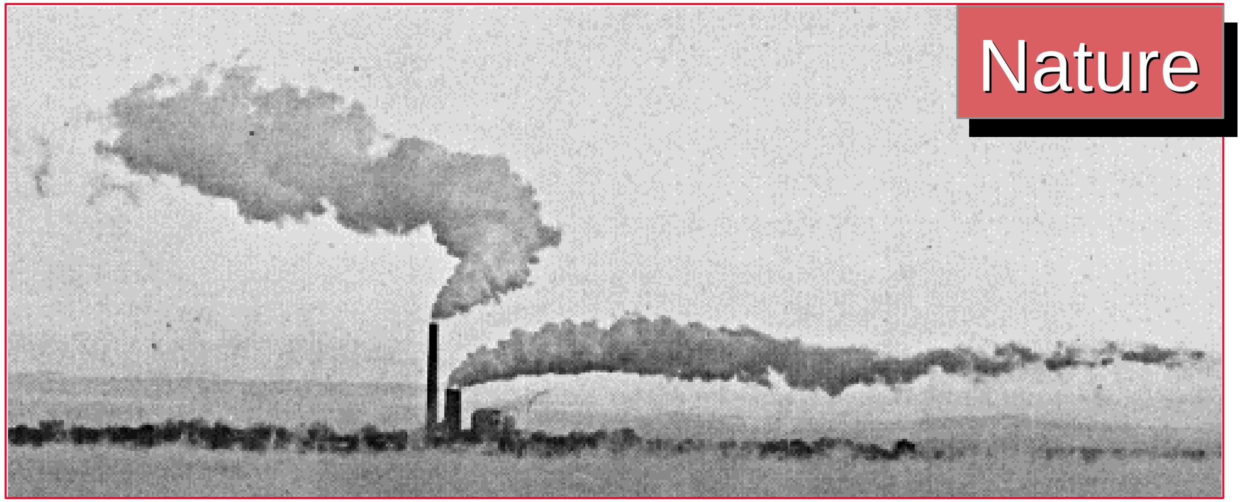
Challenges Facing the Chemical Industry

- Globalization, Competition
- Shorter Product Life Cycles
- Environmental Issues
- Emerging Technologies
- Capacity Expansions
- New Materials
- *Etc.*

All Involve Chemical Reactions

How Can The Grid Help Meet the Challenges?

Challenges - Complex Application Domains



Process Models

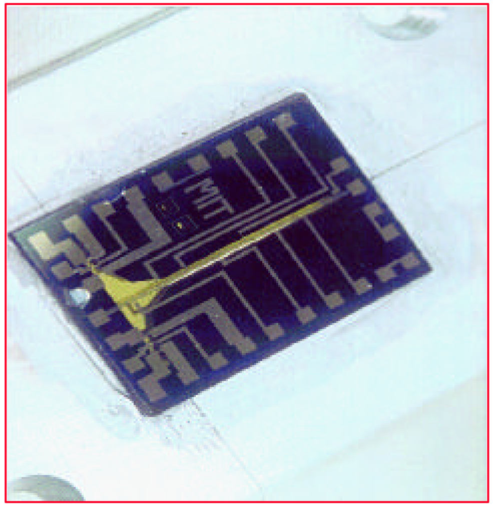
$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot \rho u^2 = -2\Omega \times \rho u - \nabla p + \nabla \cdot (\mu \nabla \cdot u)$$

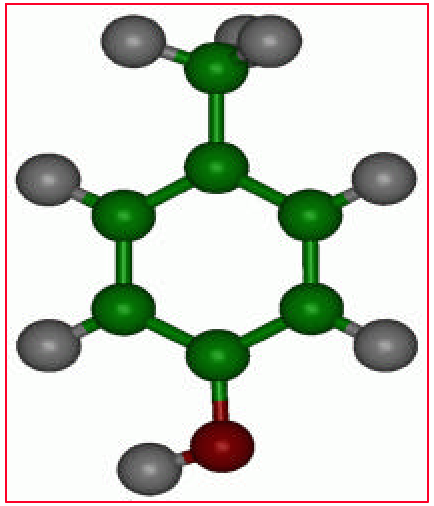
$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \rho E u = \nabla \cdot (k \nabla T) + Q_H - \nabla \cdot F^{rad} - p \nabla \cdot u$$

Challenges - The Problem of Scale

O(km)



O(cm)



O(nm)

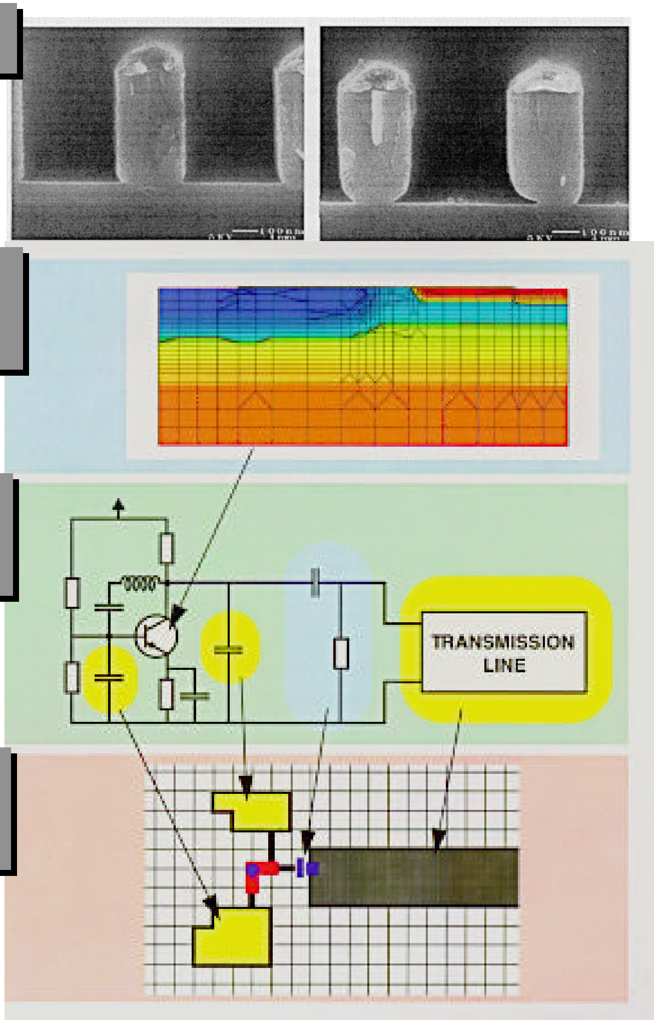
Challenges-A Hierarchy of Modeling Systems With Uncertainty Everywhere

Processing

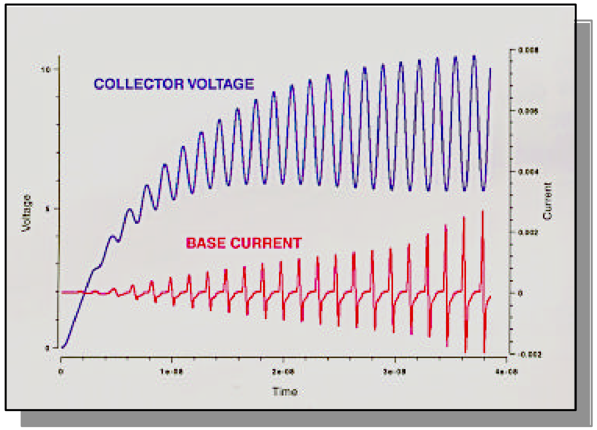
Device Model

Circuit Model

Circuit Board



Transient Response



But: What Are the Effects of Uncertainties on Performance?

Alliance Chemical Engineering AT Team

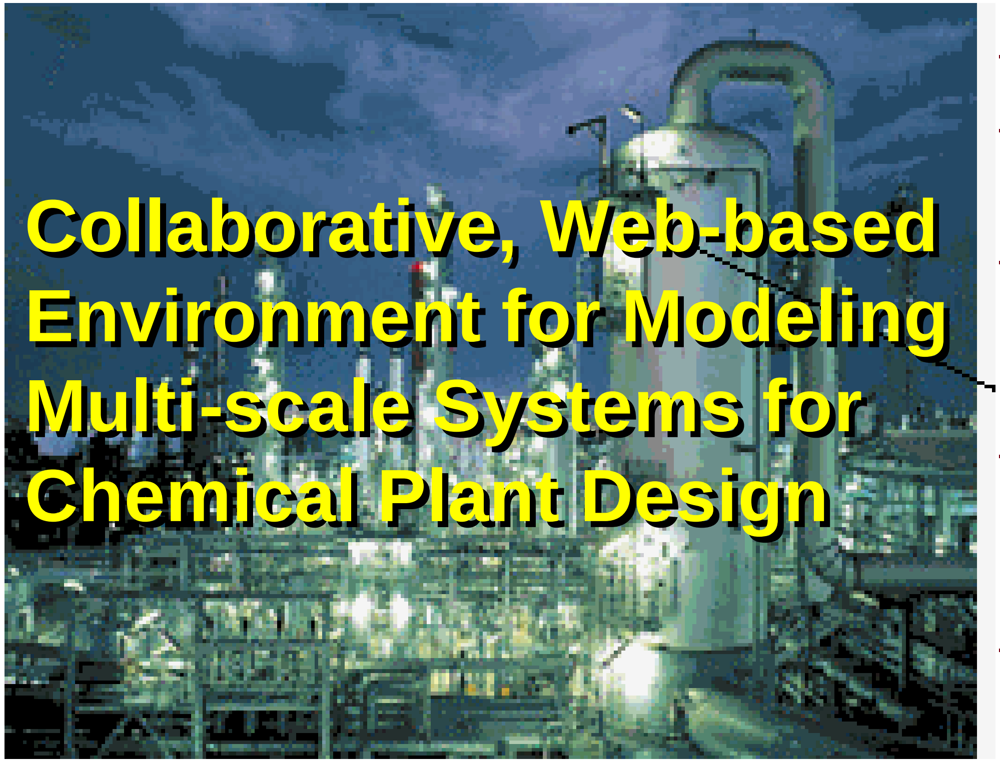
- Gregory McRae,Chairman, MIT
- Jay Alameda, NCSA
- Paul Barton, MIT
- Ken Bishop, University of Kansas
- Richard Braatz, UIUC
- Klavs Jensen, MIT
- and you!!

The Chemical Engineer's Workbench

A Computational System that::

- Provides an Integrated Environment for Process Modeling, Control, and Optimization
- Links Multiple Scales and Software Tools From Different Vendors
- Utilizes the "Best" Computing and Software Tools to Help Solve Practical Applications

Alliance Chemical Engineering Team
Developing the Chemical Engineer's Workbench



- **Web Interface for:**
  - *Ab Initio* Chemistry Calculations
  - Dynamic Chemical Process Simulations
  - Implementation of Automated Parameter Estimation and Experimental Design Algorithms
  - Link Process Simulation Packages to *Ab Initio* Codes for Physical Properties
  - Data Mining, Analysis, & Visualization
- **Testing of Prototype Workbench Using a Detailed Chemical Reactor Model**

Algorithmic Developments

- **Automatic Differentiation (ADIFOR Tool)**
  - Numerical Optimization
  - Solving Stiff ODEs/PDEs
- **Solution of Large Linear Algebra Problems**
  - Process Flowsheet Simulation
  - Parameter Estimation and Optimization
- **Solution of Integro-Partial-Differential Equations**
- **Parallel Methods for Uncertainty Analysis**

Goal-Closing the Loop to Optimize Chemical Plant Operations

Process

Measurements and Experimental Design

Process Data

Parameter Estimation

Process Model

Plant-wide Control

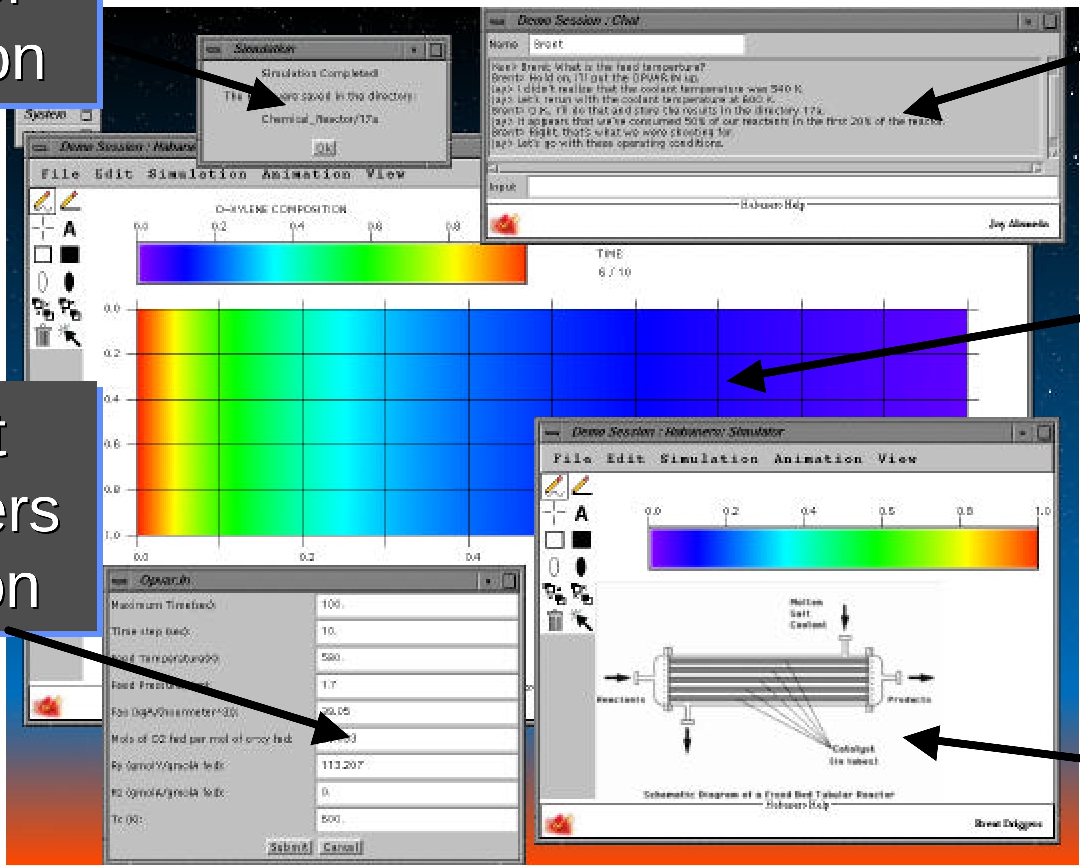
Control Signals

Grid Coupling:
- Sensors
- Networks
- Data
- HPC Models
- Controls

Goal-Create Collaborative Interface to Link Multiple Investigators With the Grid

Status of Simulation

Interactive Discussion

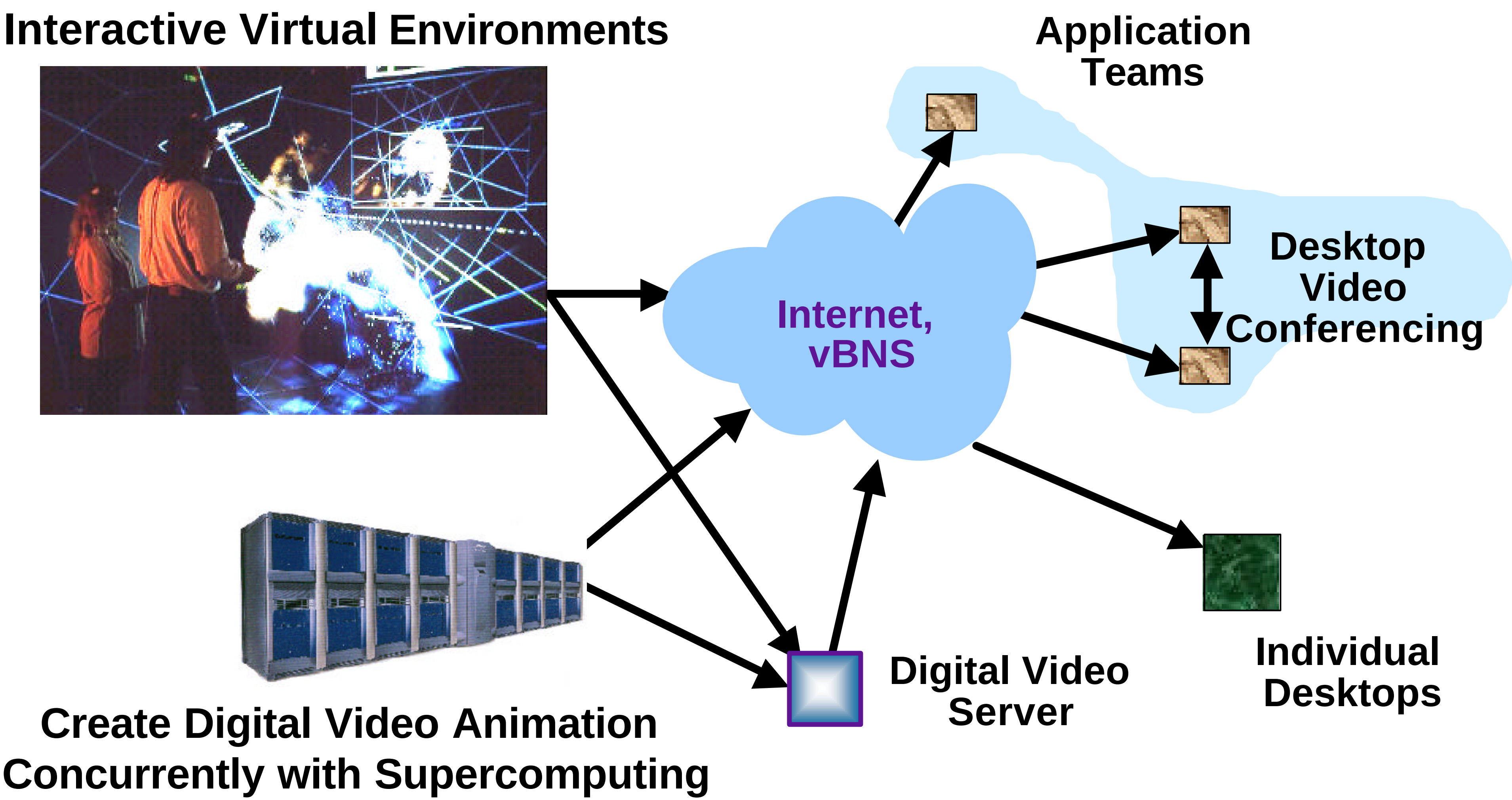


Detailed Visualization

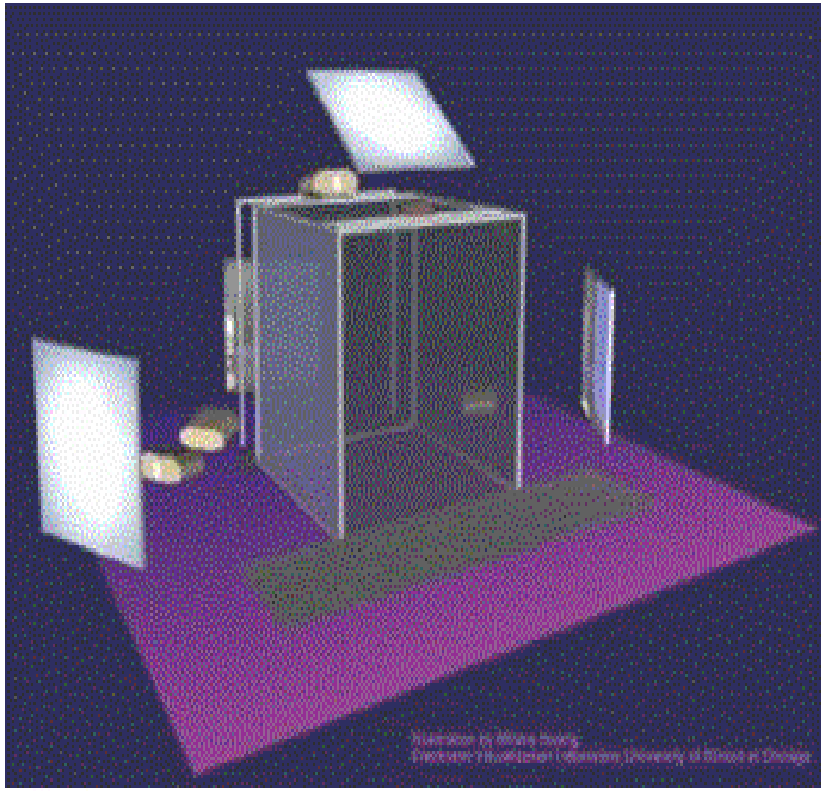
Current parameters in solution

Reactor Simulation

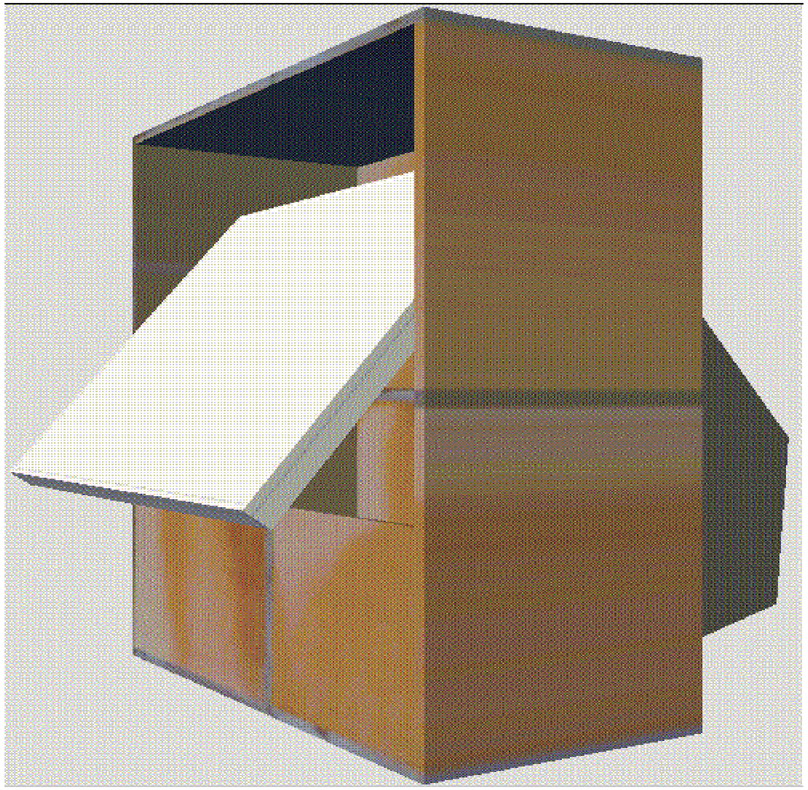
Goal-Integrating Digital Video Throughout the Enterprise



The Killer Application for the Grid - Collaborative Tele-Immersion



CAVE

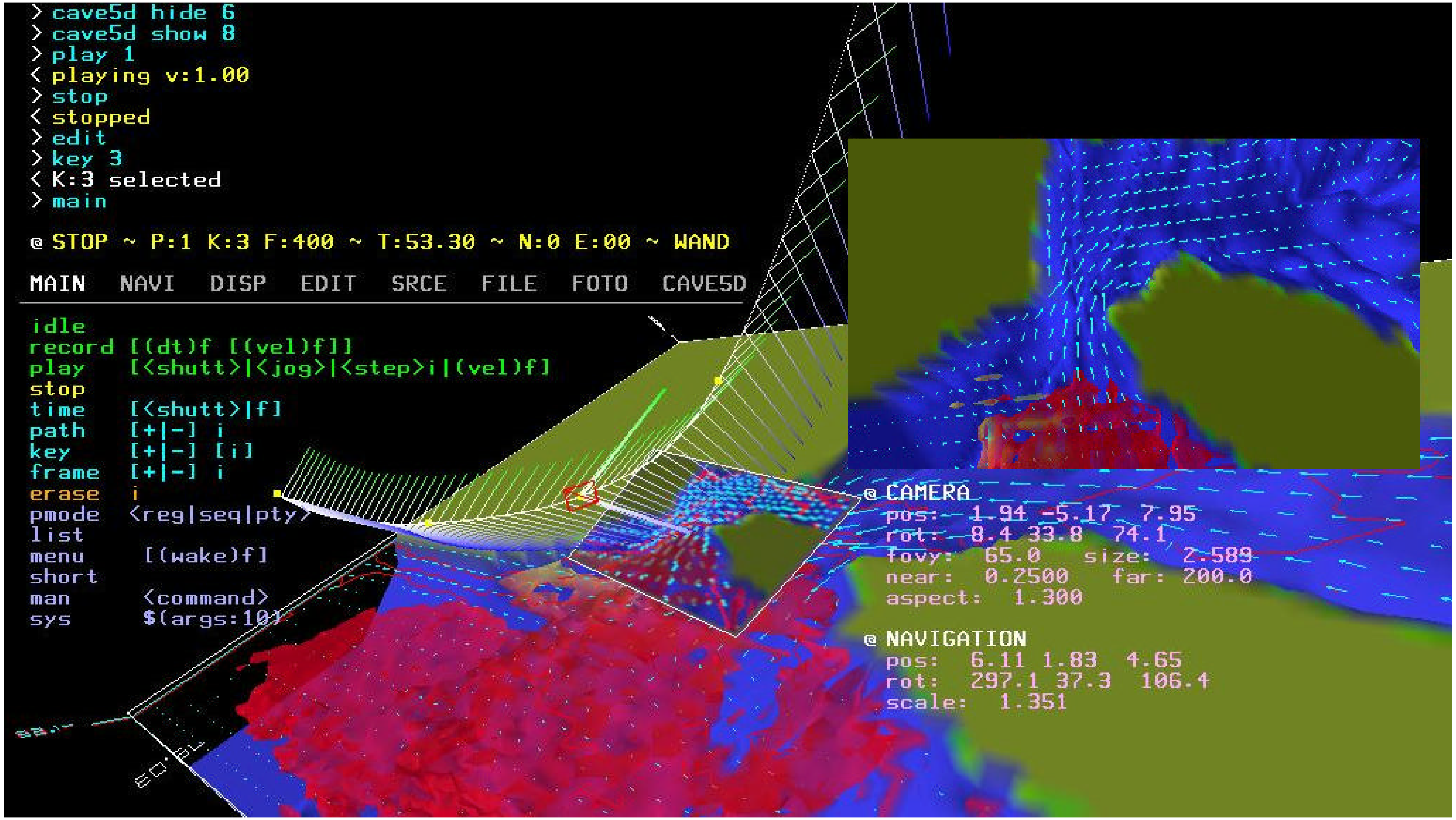


ImmersaDesk

Different Physical Implementations of the Alliance CAVE Software Libraries

Image courtesy: Electronic Visualization Laboratory, UIUC

Goal-Analyze and Record Complex Data sets Using Interactive Virtual Environments



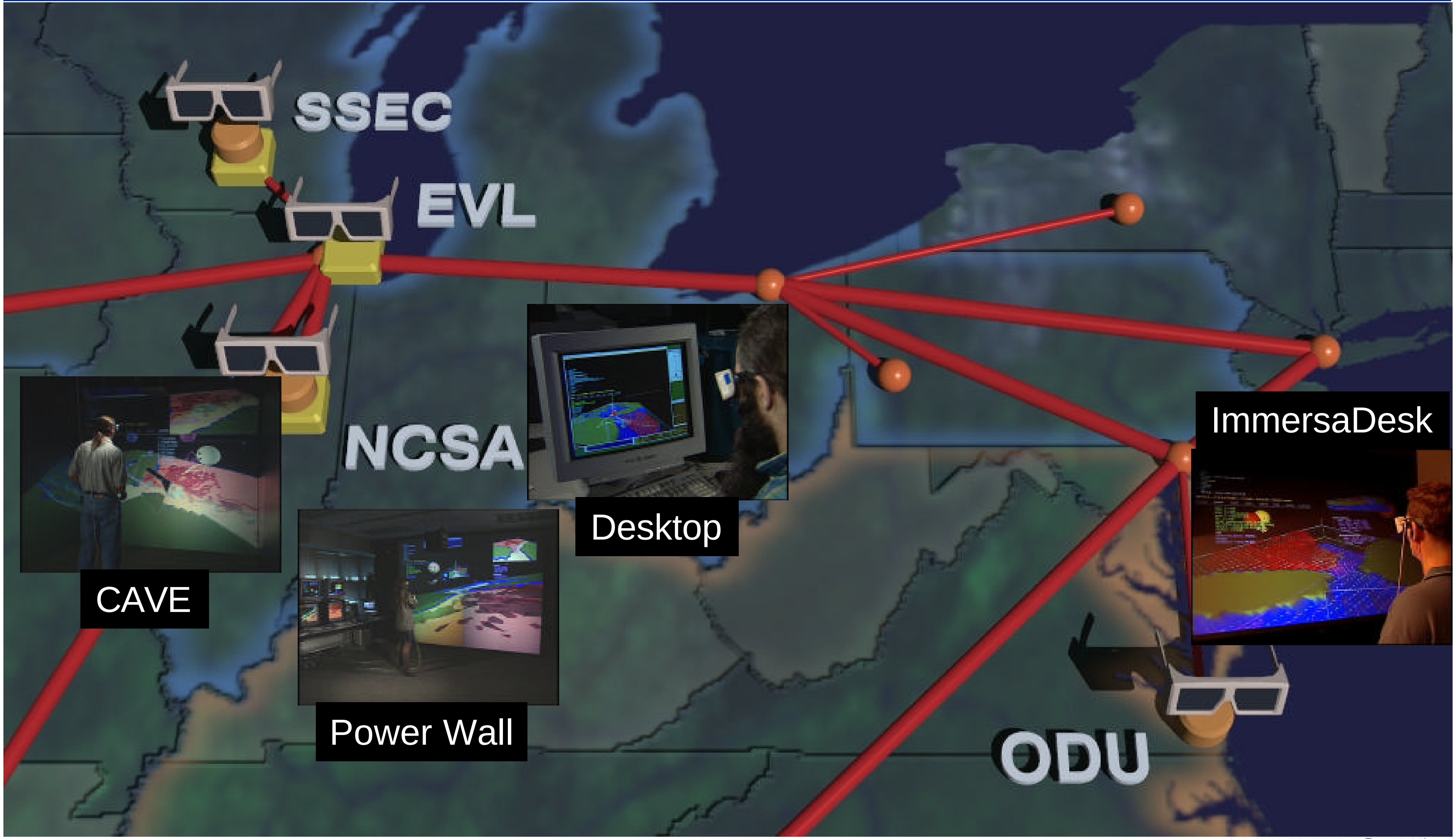
Cave5d Enables Interactive Visualizations of Time-Varying, 3-Dimensional Vis5d Data Sets in CAVE Environments

Donna Cox, Robert Patterson, Stuart Levy, NCSAVirtual Director Team
Glenn Wheless, Cathy Lascara, Old Dominion Univ.

NCSA
National Computational Science Alliance

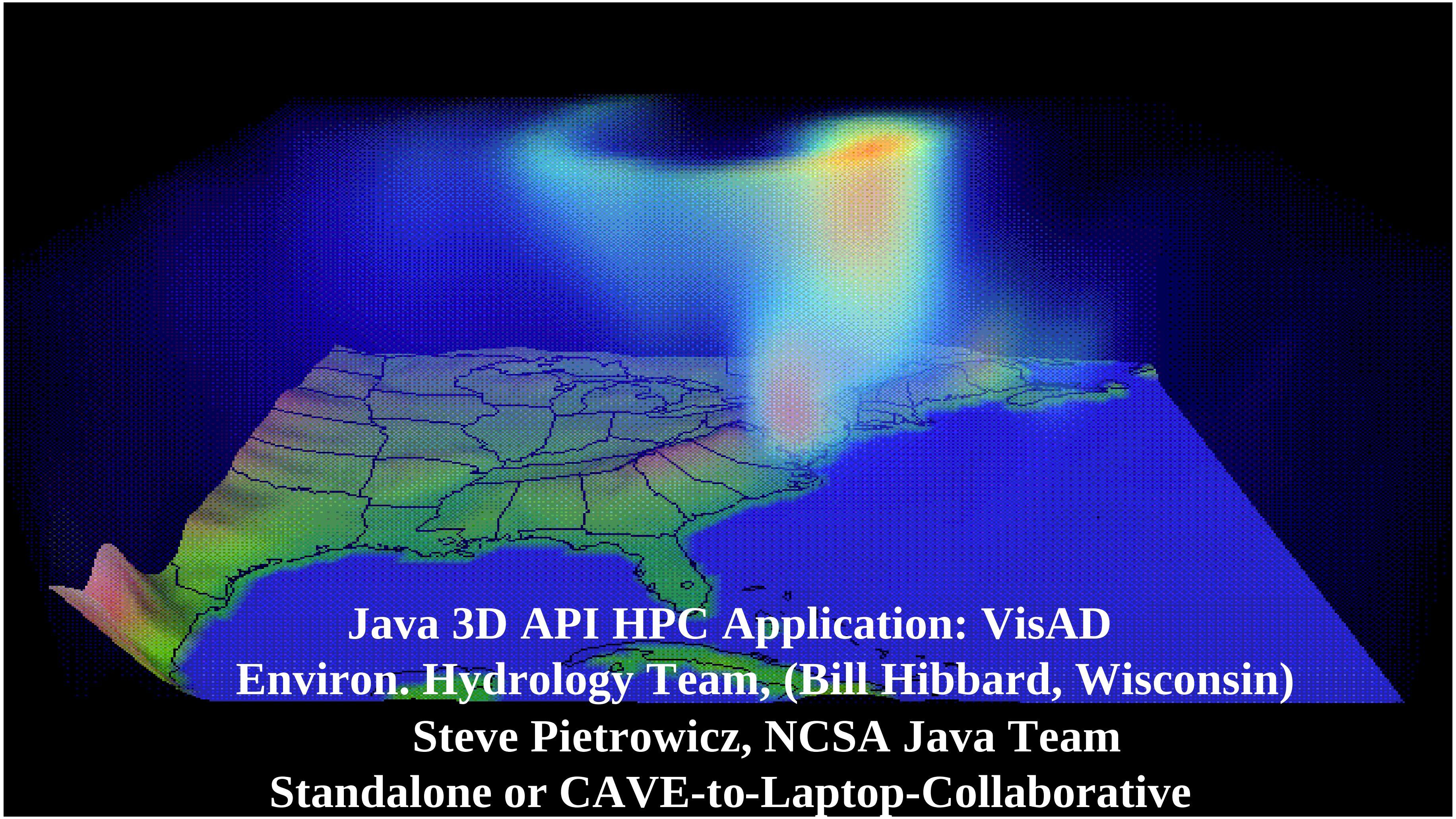
Goal-Create Shared Virtual Environment

CVD -- Collaborative Virtual Director



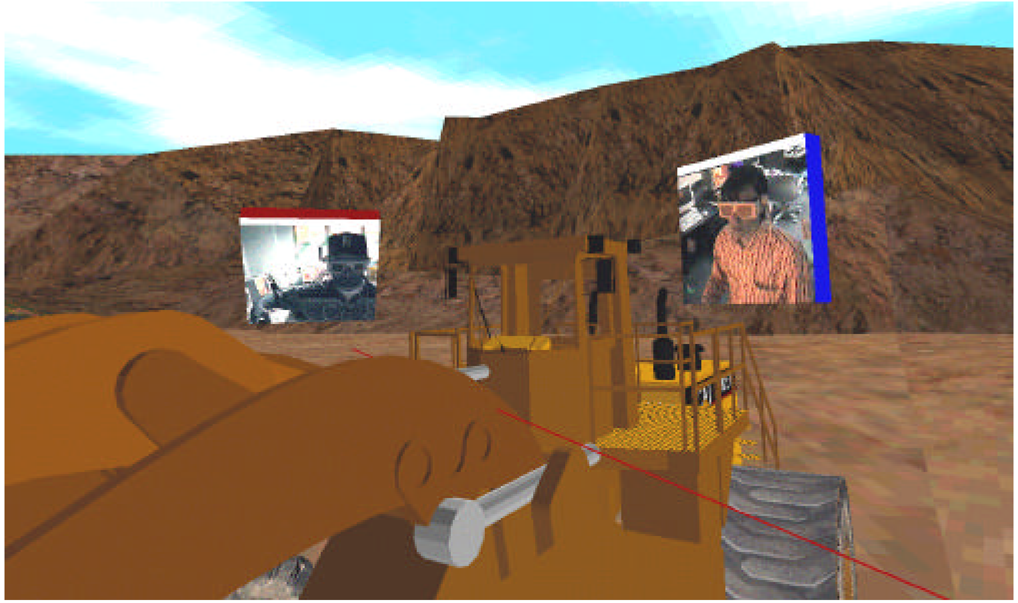
Donna Cox, Robert Patterson, Stuart Levy, NCSAVirtual Director Team
Glenn Wheless, Old Dominion Univ.

Goal-Linking the CAVE to the Desktop: Collaborative Java3D



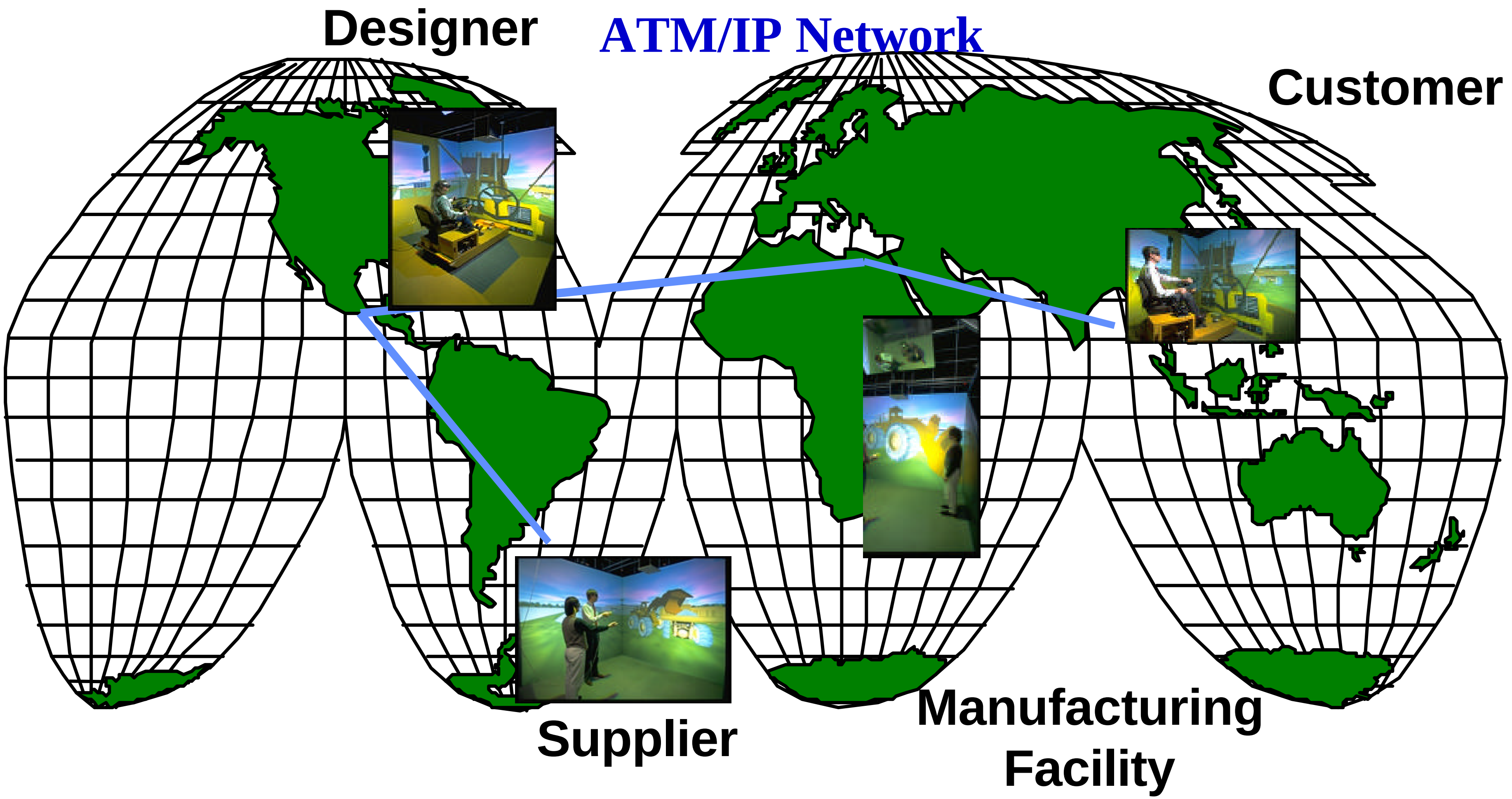
NASA IPG is Adding Funding To Collaborative Java3D

A Working Model-Caterpillar's Collaborative Virtual Prototyping Environment

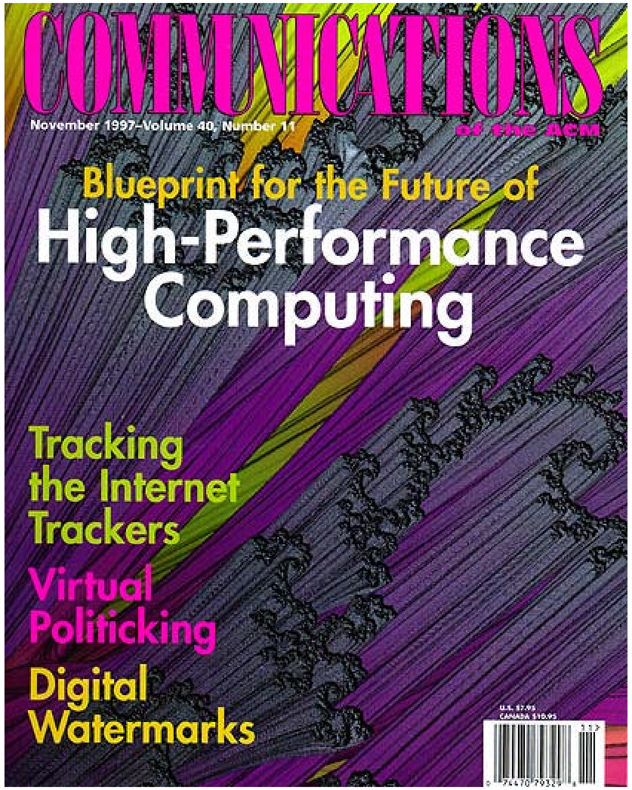


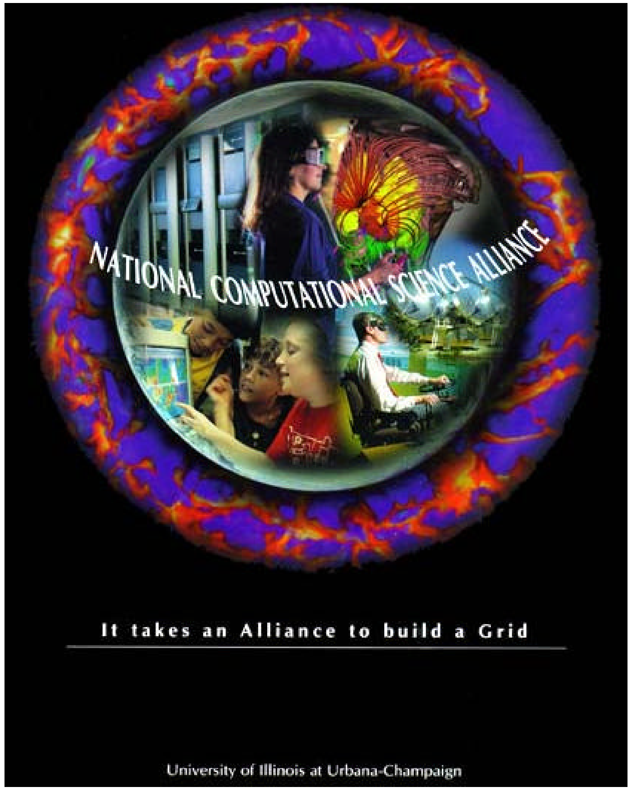
Real Time Linked VR and Audio-Video
Between NCSA and Germany
Using SGI Indy/Onyx and HP Workstations

Goal-Global Enterprise Management



How to Find Out More About the Alliance





See also http://alliance.ncsa.uiuc.edu