

# Grid Computing

*Dr Simon See  
High Performance Computing  
Sun Microsystems Inc*

# The Grid

## BLUEPRINT FOR A NEW COMPUTING INFRASTRUCTURE

“The grid is an emerging *infrastructure* that will fundamentally change the way we think about – and use – computing. The grid will... create a universal source of computing power.”

# Grid Computing

ARCHITECTURE, IMPLEMENTATION AND  
MANAGEMENT.

- Historical Perspective
- Industry Characteristics
- Requirements and Policies
- Architecture
- Implementation
- Usability and Management
- Extensibility and Web Services

# Definitions

## Grid Computing Environments



**Compute Farm**

**Cluster**

**Grid**

A Grid is a hardware/software/instruments/service infrastructure that provides **dependable, consistent, pervasive, inexpensive** \* access to computational and data capabilities.

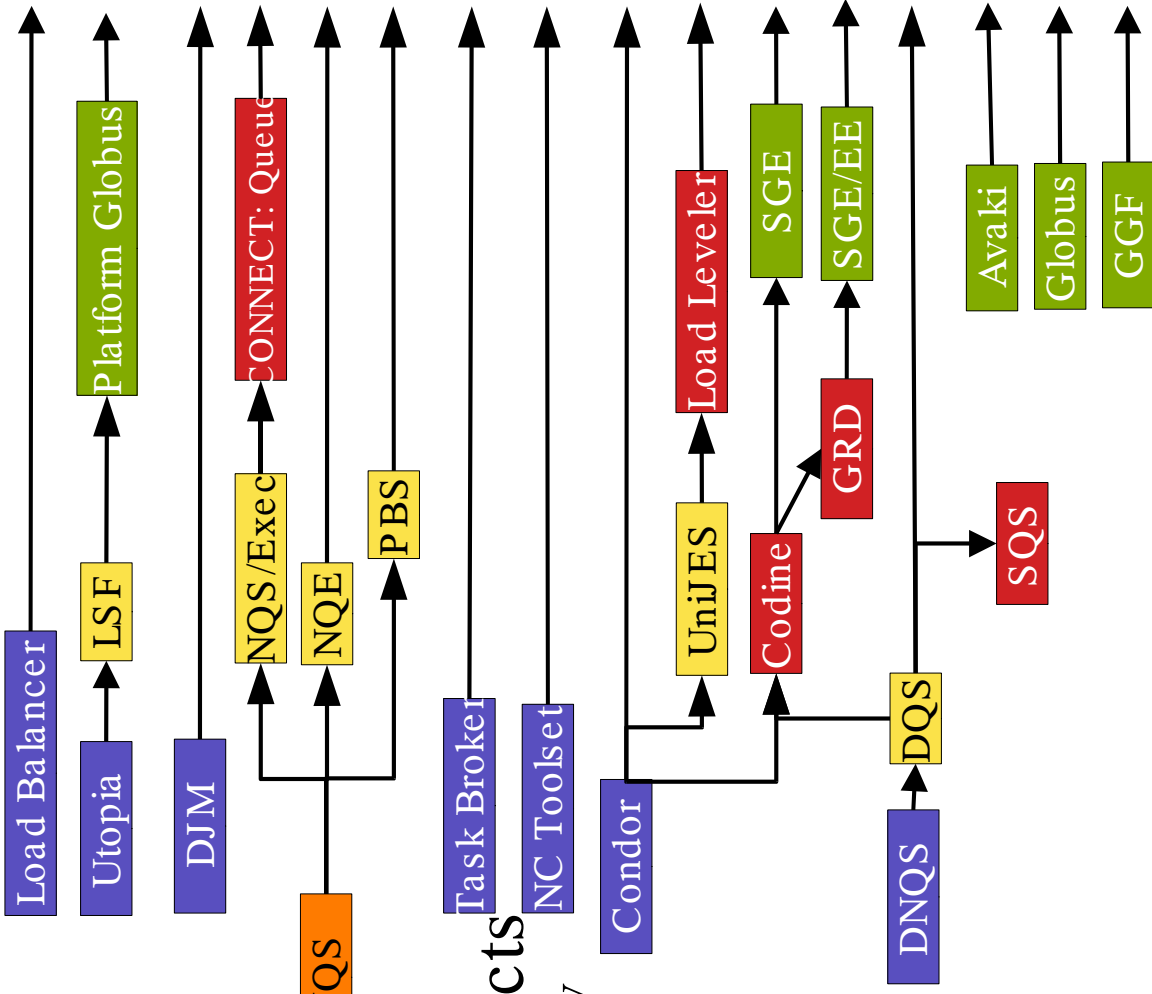
\* Foster, Kesselman, 1999

# Definitions

## Grid Computing Environments

- Distributed Resource Management
  - SGE
  - LSF
  - NQS
  - DJJM
- Parallel Computing Environments
  - PVM
  - MPL
  - MPI
  - FORTRAN 90
  - Linda

# Grid Computing Genealogy



- **Early Grid Technologies**

- Distributed Job Manager; DJM
- Network Queuing System: NQS
- University Research projects

- **Mature Commercial Products**

- Sun Grid Engine (Sun, formerly Codine/GRD)
- Load Sharing Facility (Platform Computing)
- Load Leveler

- **Industry Collaboration / Leadership**

- Globus
- Global Grid Forum
- Platform Globus

# Industry Characteristics

## Life

### Scientific

- **Low cost efficient**
- **Custom research or limited use applications**
- **Multi-day application runs (BLAST)**
- **Exponential Combinations**
- **Limited administrative staff**
- **Complementary techniques**

### Financial

### Services

- **Market simulations**
- **Time IS Money**
- **Proprietary applications**
- **Multiple Platforms**
- **Multiple scenario execution**
- **Need instant results and analysis tools**

## Electronic

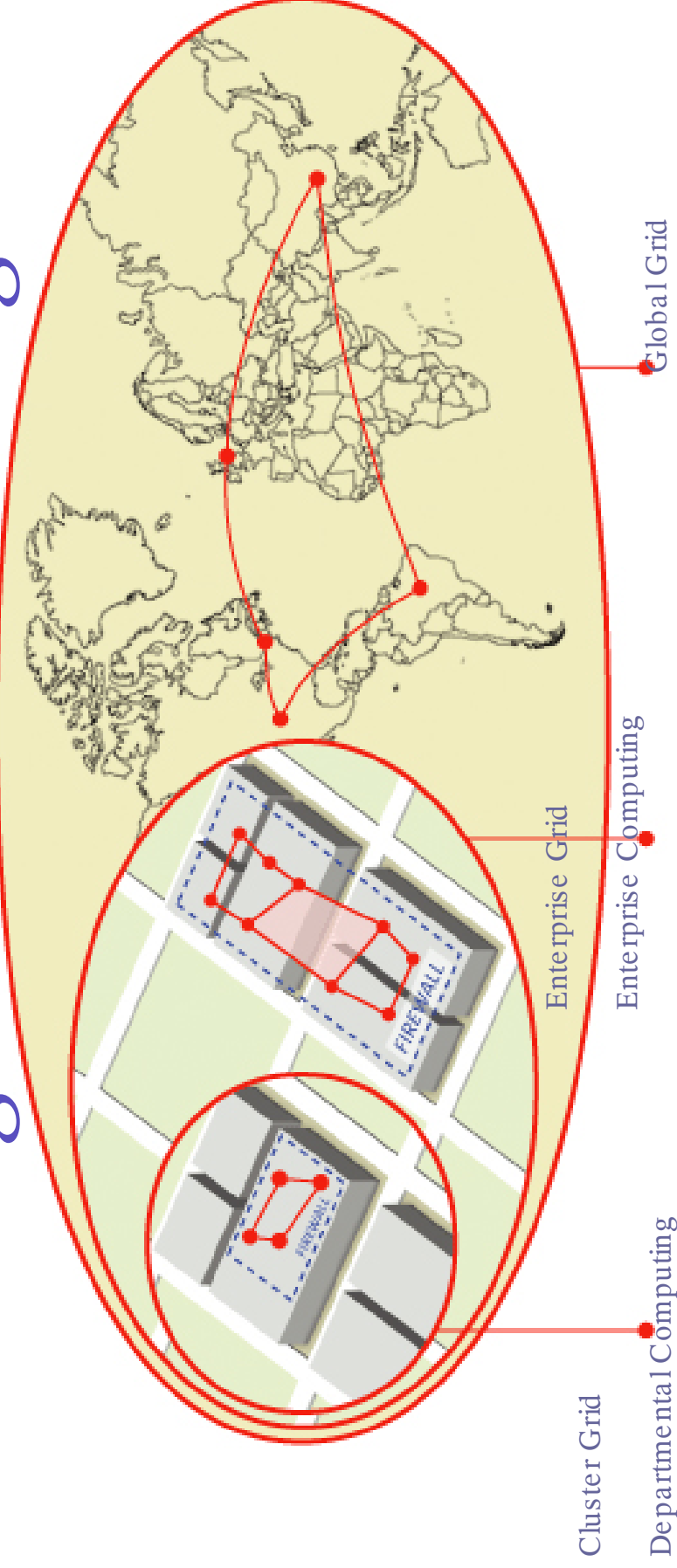
### Design

- **Time to Market**
- **Fastest platforms, largest Grids**
- **License Management**
- **Well established application suite**
- **Large legacy investment**
- **Platform Ownership issues**

## High Performance Computing

- **Parallel Reservoir Simulations**
- **Geophysical Ray Tracing**
- **Custom in-house codes**
- **Well established application suite**

# Grid Evolutionary Strategy: starting with the cluster grid



Internet Computing

- Simplest Grid deployment
- Maximum utilization of departmental resources
- Resources allocated based on priorities
- Resources shared within the enterprise
- Policies ensure computing on demand
- Gives multiple groups seamless access to enterprise resources
- Resources shared over the Internet
- Global view of distributed datasets



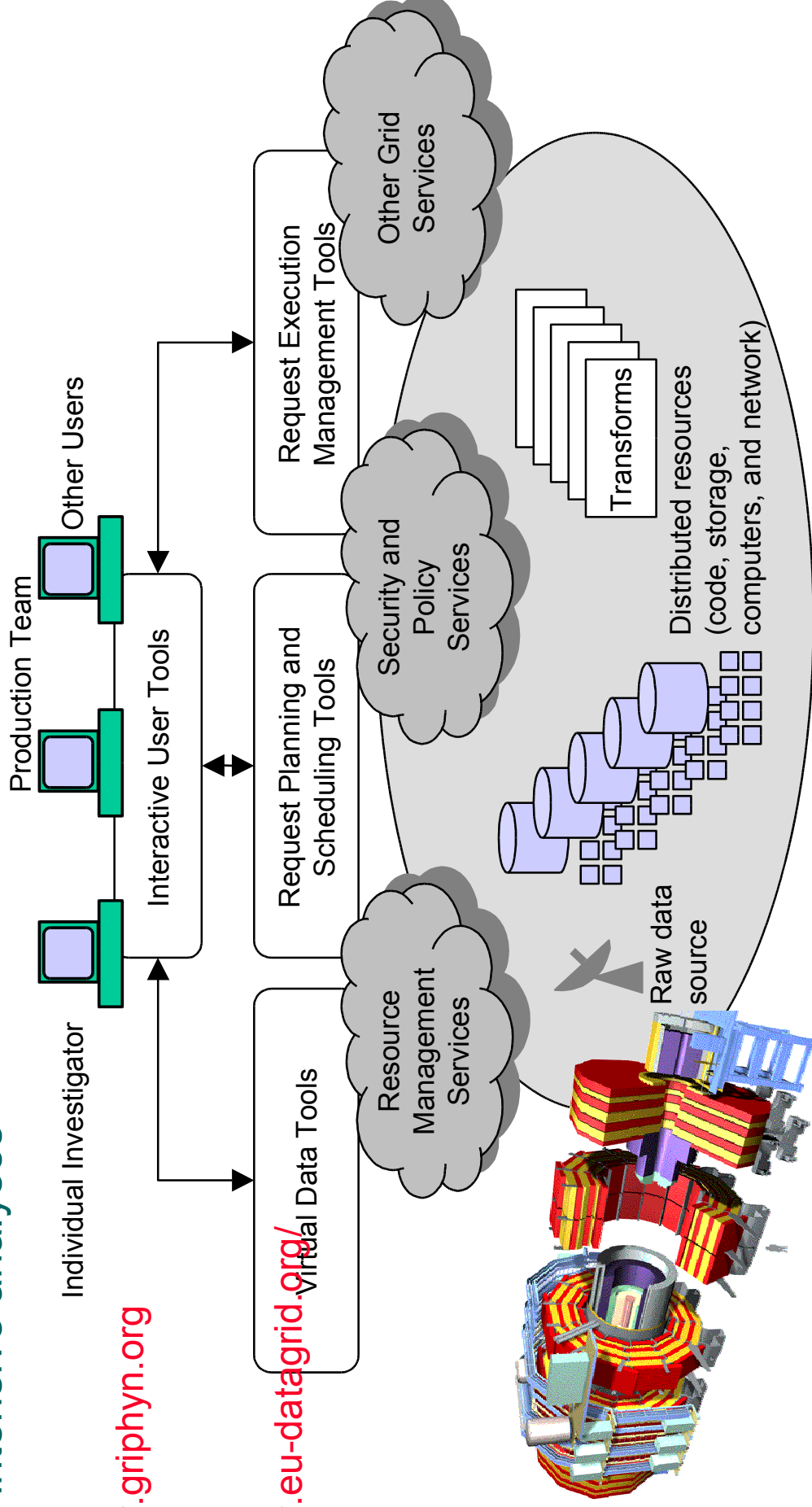
# Example Grid Communities

## •GriPhyN and European DataGrid

- Enable (thousands of) physicists to pool data & computing resources for data-intensive analyses

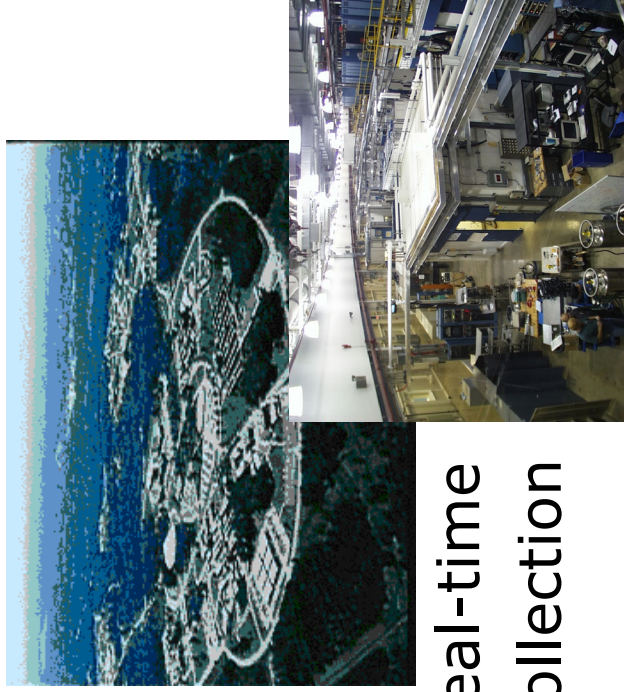
<http://www.griphyn.org>

<http://www.eu-datagrid.org>



# Online Access to Scientific Instruments

Advanced Photon Source

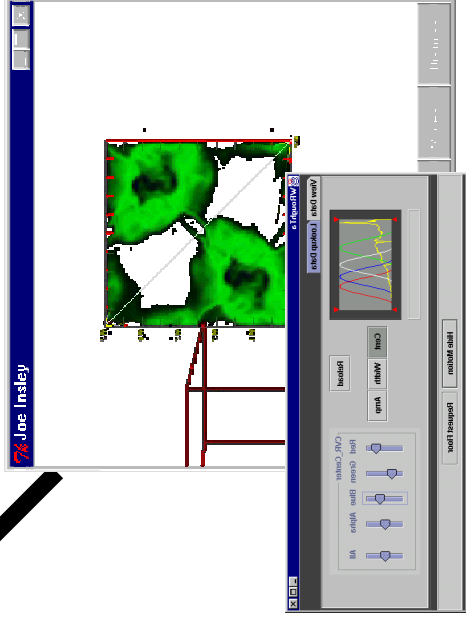


real-time collection

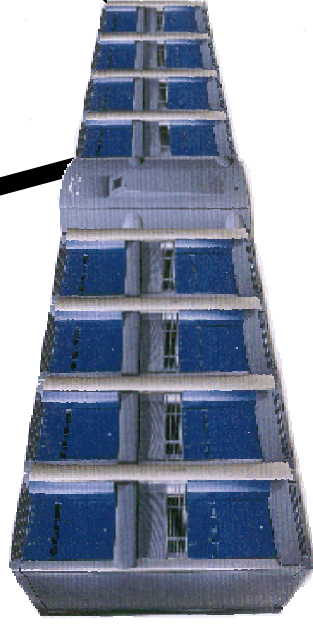
wide-area dissemination



desktop & VR clients with shared controls



archival storage



tomographic reconstruction

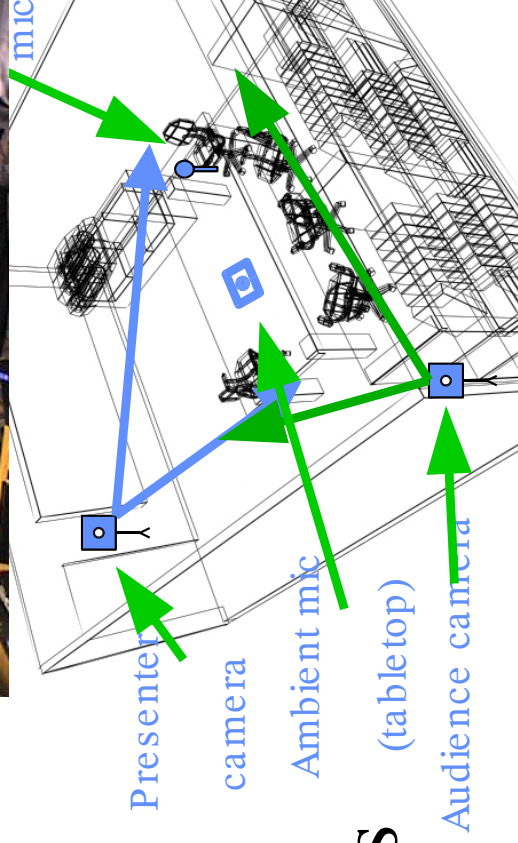
# Example Grid Communities



- Access Grid
- Collaboration
  - Enable collaborative work at dozens of sites worldwide, with strong sense of shared presence
  - Combination of commodity audio/video tech + Grid technologies for security, discovery, etc.

<http://www.accessgrid.org>

- 40+ sites worldwide, number rising rapidly



# The Grid Problem

- Flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resource

From “The Anatomy of the Grid: Enabling Scalable Virtual Organizations”

- Enable communities (“virtual organizations”) to share geographically distributed resources as they pursue common goals -- *assuming the absence* of...
  - central location,
  - central control,
  - omniscience,
  - existing trust relationships.

# Elements of the Problem

- Resource sharing
  - Computers, storage, sensors, networks, ...
  - Sharing always conditional: issues of trust, policy, negotiation, payment, ...
- Coordinated problem solving
  - Beyond client-server: distributed data analysis, computation, collaboration, ...
- Dynamic, multi-institutional virtual orgs
  - Community overlays on classic org structures
  - Large or small, static or dynamic

# Data Grids for High Energy Physics



1 TIPS is approximately 25,000 Spec.Int95 equivalents

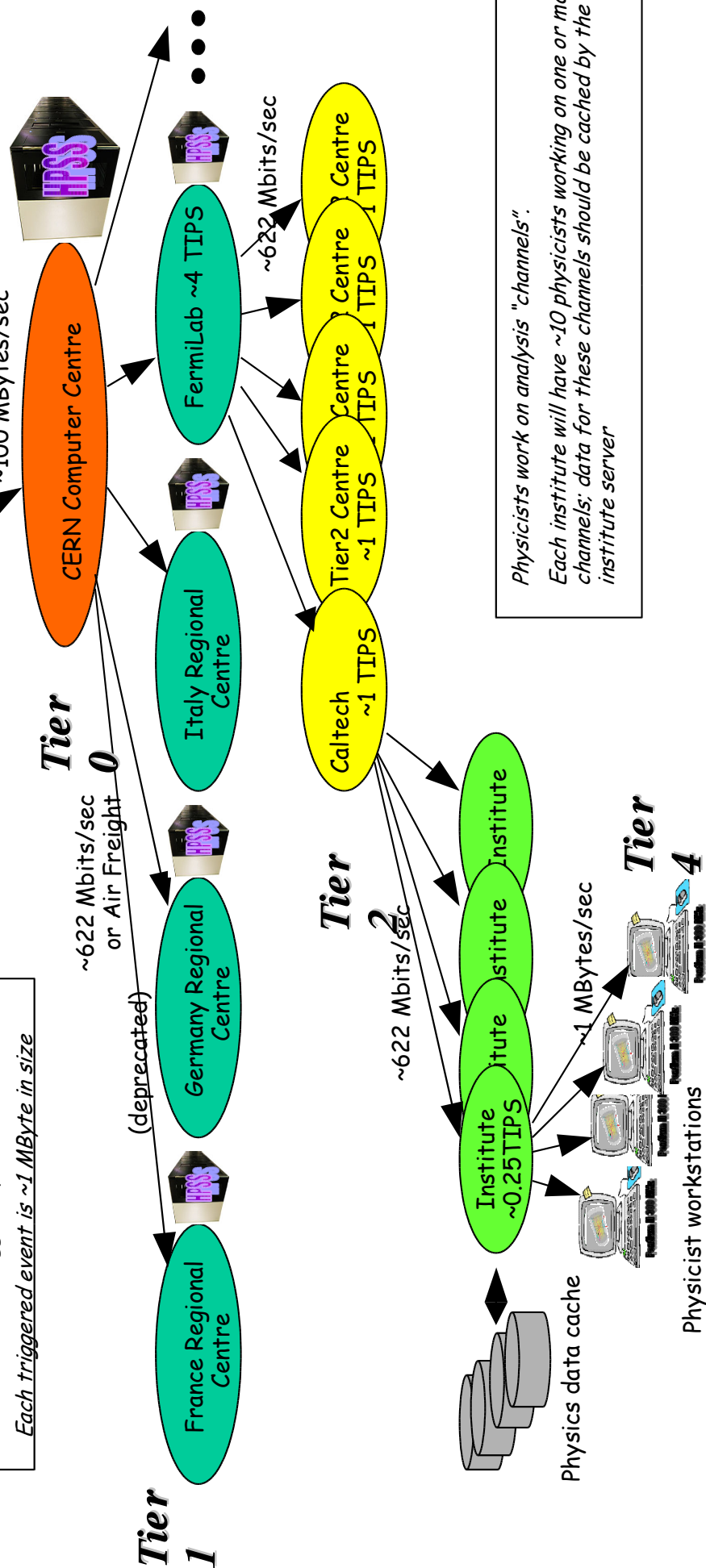
There is a "bunch crossing" every 25 nsecs.  
 There are 100 "triggers" per second  
 Each triggered event is ~1 MByte in size

~100 MBytes/sec

Offline Processor Farm

~20 TIPS

~100 MBytes/sec

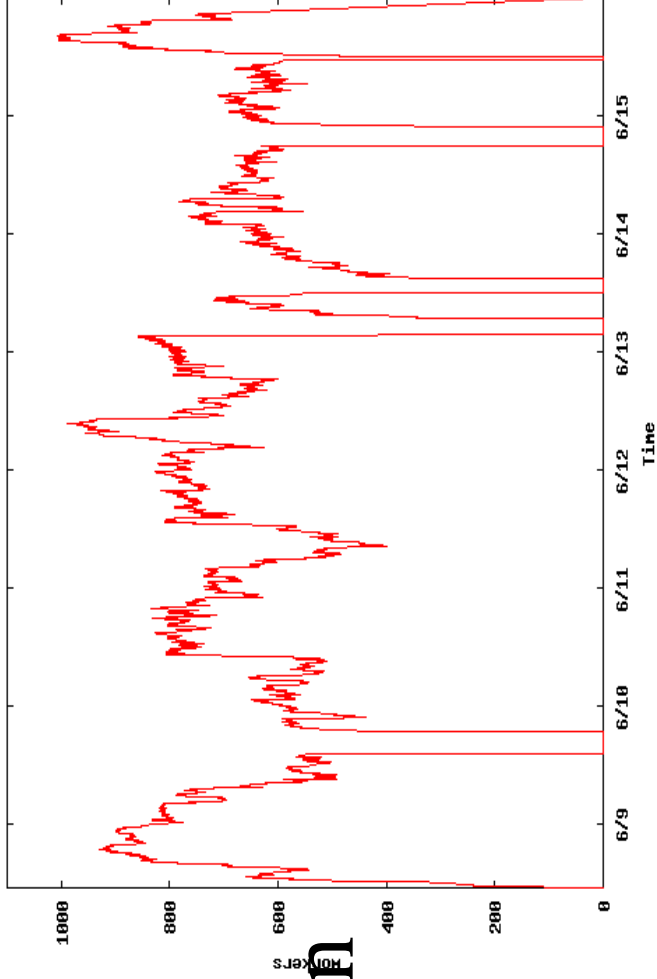


Physicists work on analysis "channels".  
 Each institute will have ~10 physicists working on one or more channels; data for these channels should be cached by the institute server

Image courtesy Harvey Newman, Caltech

# Mathematicians Solve NUG30

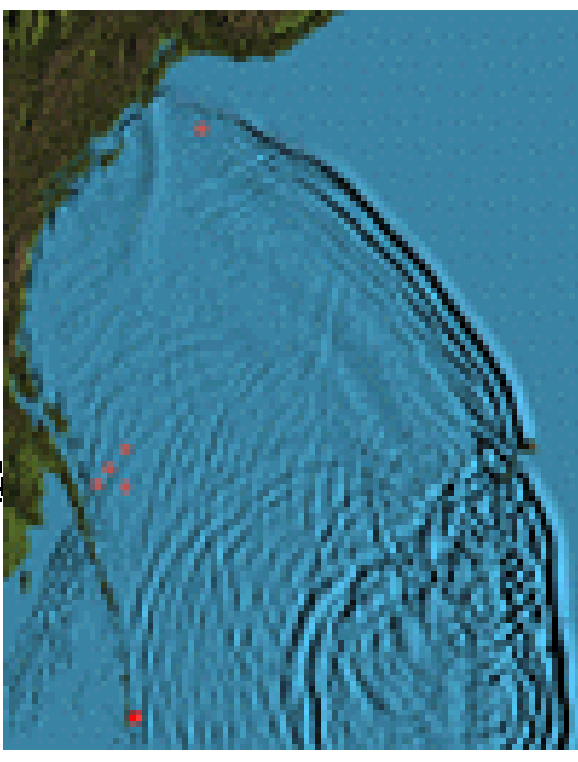
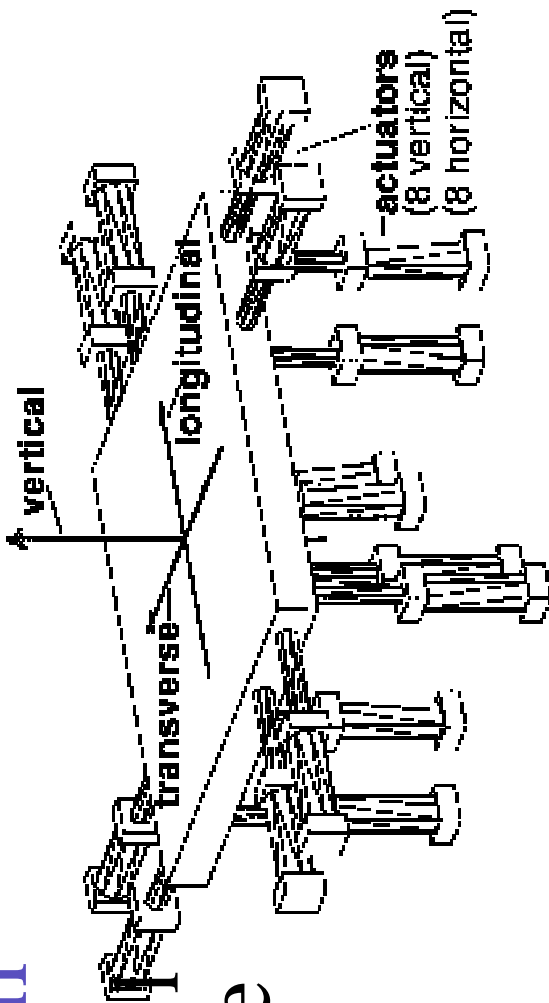
- Looking for the solution to the NUG30 quadratic assignment problem
- An informal collaboration of mathematicians and computer scientists
- Condor-G delivered 3.46E8 CPU seconds in 7 days (peak 1009 processors) in U.S. and Italy (8 sites)



MetaNEOS: Argonne, Iowa, Northwestern, Wisconsin

# Network for Earthquake Engineering Simulation

- NEESgrid: US national infrastructure to couple earthquake engineers with experimental facilities, databases, computers, & each other
- On-demand access to experiments, data streams, computing, archives, collaboration



NEESgrid: Argonne, Michigan, NCSA, UIUC, USC



# Home Computers Evaluate AIDS Drugs



- Community =
  - 1000s of home computer users
  - Philanthropic computing vendor (Entropia)
  - Research group (Scripps)
- Common goal= advance AIDS research

**fight AIDS @home** the Olson laboratory at The Scripps Research Institute computing toward a cure

powered by **entropia**

- ▶ [Fight AIDS @ Home](#)
- ▶ [The AIDS Crisis](#)
- ▶ [How Your PC can Help](#)
- ▶ [Project Status](#)
- ▶ [Get the Download](#)
- ▶ [Research Team](#)
- ▶ [The Discovery Research Team](#)
- ▶ [Links and Communities](#)
- ▶ [Entropia](#)
- ▶ [Link Your Site to FA@H](#)
- ▶ [FAQ](#)

**Free Software for Your PC** - By [downloading Entropia](#) onto your PC, [FightAIDS@Home](#) uses your computer's idle resources to accelerate powerful new anti-HIV drug design research!

**FightAIDS@Home** is a computational research project conducted by the [Olson laboratory at The Scripps Research Institute](#) in La Jolla, California. The project uses Entropia's global Internet computing grid, which runs both commercial and research applications on PCs.

**How Your PC Helps - FightAIDS@Home** uses your computer to generate and test millions of candidate drug compounds against detailed models of evolving HIV viruses, a feat previously impossible without dozens of multi-million dollar supercomputers. Every PC matters!

September 22, 2000

# Broader Context

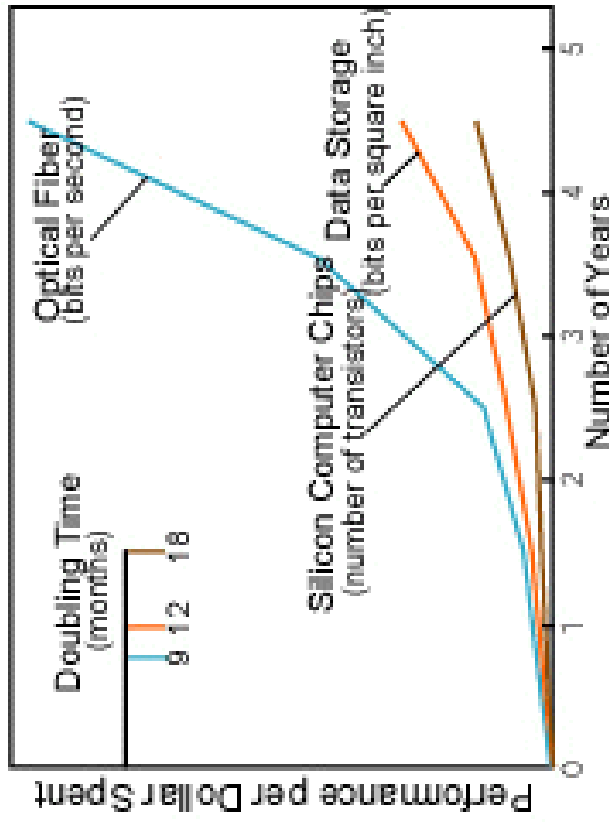
- “Grid Computing” has much in common with major industrial thrusts
  - Business-to-business, Peer-to-peer, Application Service Providers, Storage Service Providers, Distributed Computing, Internet Computing...
- Sharing issues not adequately addressed by existing technologies
  - Complicated requirements: “run program X at site Y subject to community policy P, providing access to data at Z according to policy Q”
  - High performance: unique demands of advanced & high-performance systems

# Why Now?

- Moore's law improvements in computing produce highly functional end systems
- The Internet and burgeoning wired and wireless provide universal connectivity
- Changing modes of working and problem solving emphasize teamwork, computation
- Network exponentials produce dramatic changes in geometry and geography

# Network Exponentials

- Network vs. computer performance
  - Computer speed doubles every 18 months
  - Network speed doubles every 9 months
  - Difference = order of magnitude per 5 years
- 1986 to 2000
  - Computers: x 500
  - Networks: x 340,000
- 2001 to 2010
  - Computers: x 60
  - Networks: x 4000



**Moore's Law vs. storage improvements vs. optical improvements.** Graph from **Scientific American** (Jan-2001) by Cleo Vilett, source Vined Khoslan, Kleiner, Caufield and Perkins.

# Business Drivers

- **Reduced Costs**
  - Efficient use of resources, TCO, ROI
  - Utilize latent cycles
- **Shorten Time to Market**
- **Improve business decisions, reduce risk**
- **Faster, Better, Cheaper**
- **New Capabilities, improved quality, innovation**

# Application Requirements

- **Basic Information**
  - Primary stakeholders
  - Operating Systems and support mechanisms
  - Deployment model
  - I/O and data requirements
- **Execution Profile**
  - Dynamic memory allocation, footprint
  - Performance characteristics, reference benchmarks
  - Network I/O
  - Job duration characteristics
  - Utilization trends
- **Application Characteristics**
  - Dependencies
  - Priorities vs. other applications
  - Data Management post execution
  - Checkpointing capable

# Application Stack



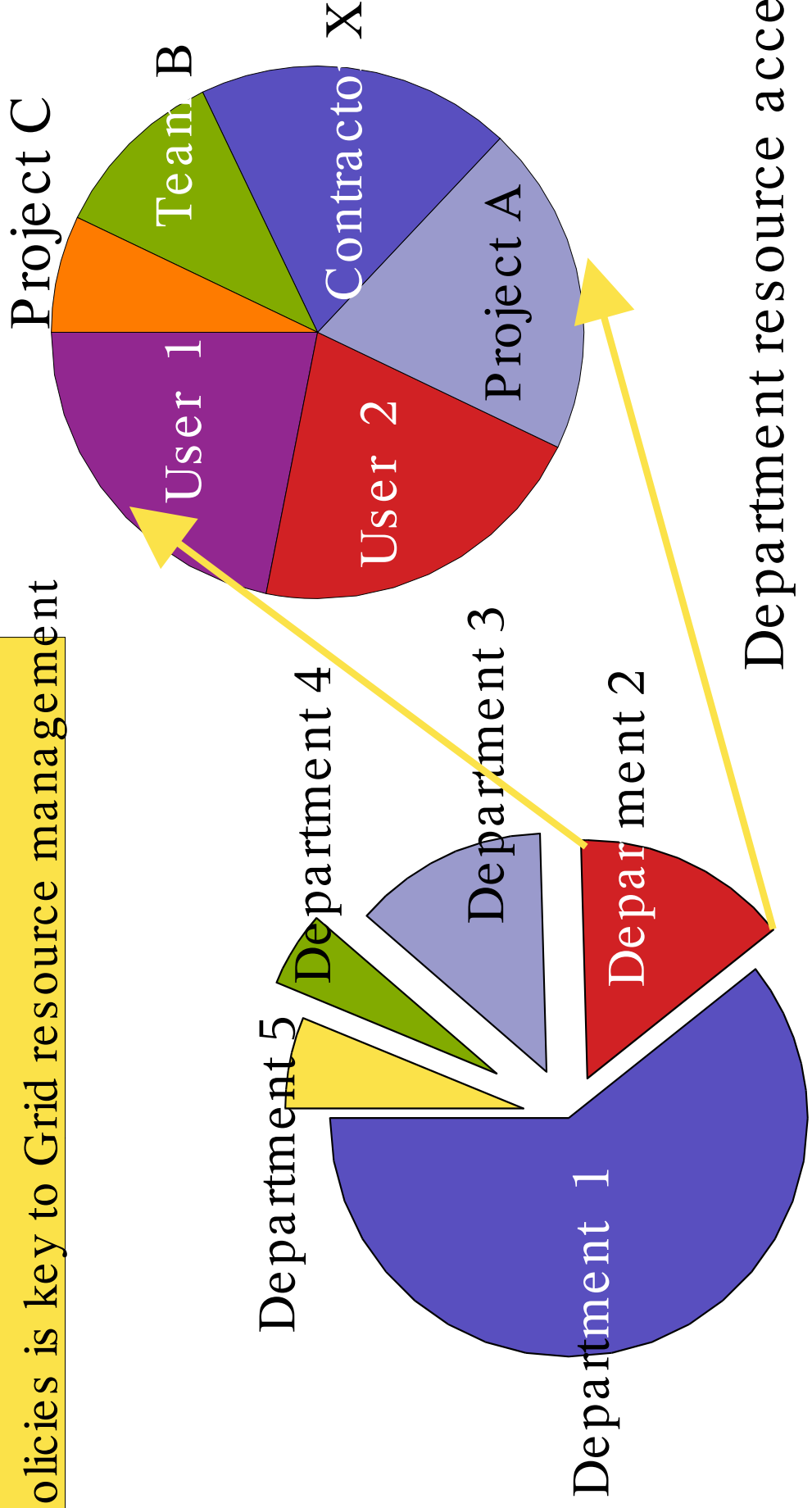
# Architectural Requirements

- **Availability**
  - Downtime impact of Grid environment
  - Impact of interruption of individual jobs
  - Acceptable maintenance windows
- **Scalability**
  - Anticipated growth over 1–3–5 years
  - Desired scaling strategy and response to peak loads
  - Strategy for technology refresh, evolution
- **Manageability**
  - Skill set/workload of administration personnel
  - Expected stability of applications
  - Code management, software distribution mechanisms
- **Security**
  - User authentication mechanisms
  - Internet access to grid
  - Data Security requirements



# Grid Policy Management

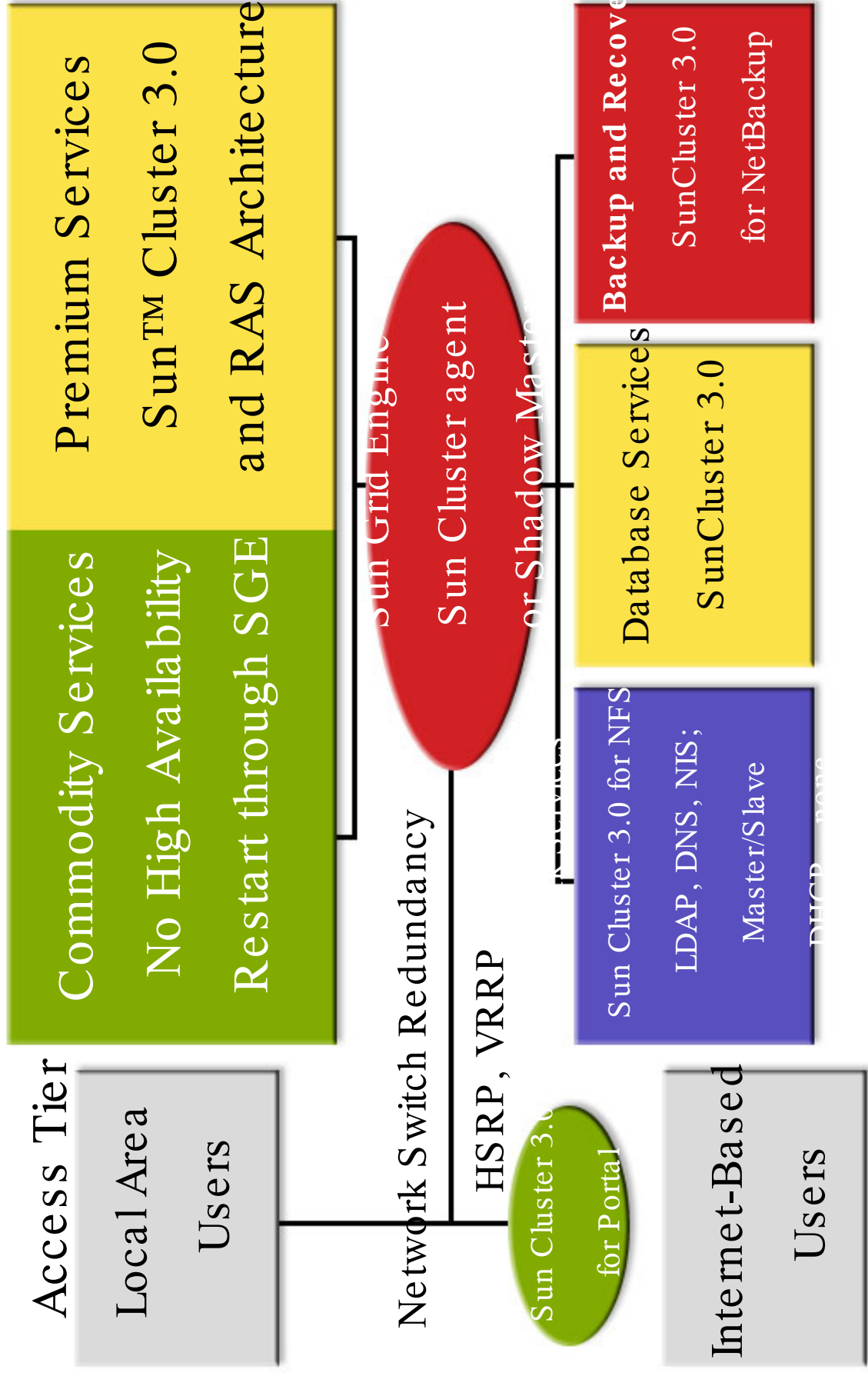
Clear definition and documentation of priorities and policies is key to Grid resource management



Campus wide resource demand

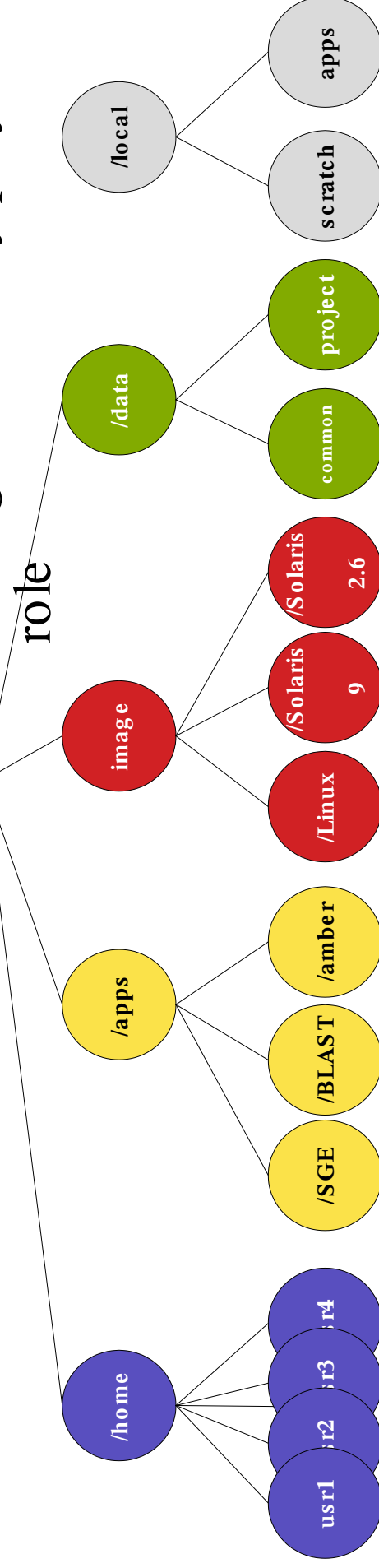
Department resource access

# Availability Model



# Data Model

- Network File System
  - Dominates Grid Environments
  - Naming Service
  - automounter
- Key to efficient deployment and management
- SAN Technologies usually present behind data service
- Local caching and data management may play a role



# Scalability

- Network architecture constrains grid scalability
- NFS Architecture scales w/ support of SAN + Server Technologies
- Scalability Model
  - Network Architecture
  - Storage Architecture
  - Operations Model

# Security

- Grid Security lays on top of existing Security architecture, good or bad
- Security Issues
  - Grid may contains resources owned by different distrustful organizations
  - Data needs to get in/out of the grid
  - Users need access to the grid
  - Insecure protocols such as NFS and automount
- Security Requirements
  - Single sign-on
  - Protection of Credentials
  - Interoperability w/ local security standards
  - Secure communication
  - Multiple implementations

# Security Recommendations

- Understand Security Policy
  - Multiple Trust domains, policy domains
  - Access from employees, partners, customers
  - Sensitivity of data, information, resources, communication
- Secure the Environment
- Security architecture techniques
  - Apply to Grid Service Infrastructure
  - Segregate the Grid from external networks with Fire walls
  - Harden operating system on Grid Nodes
- Authentication / Authorization
  - Enforce access to the Grid
  - Authorization at the user/group level
- Do not allow users direct connection to the grid nodes
- Develop secure data transfer

# Additional Requirements

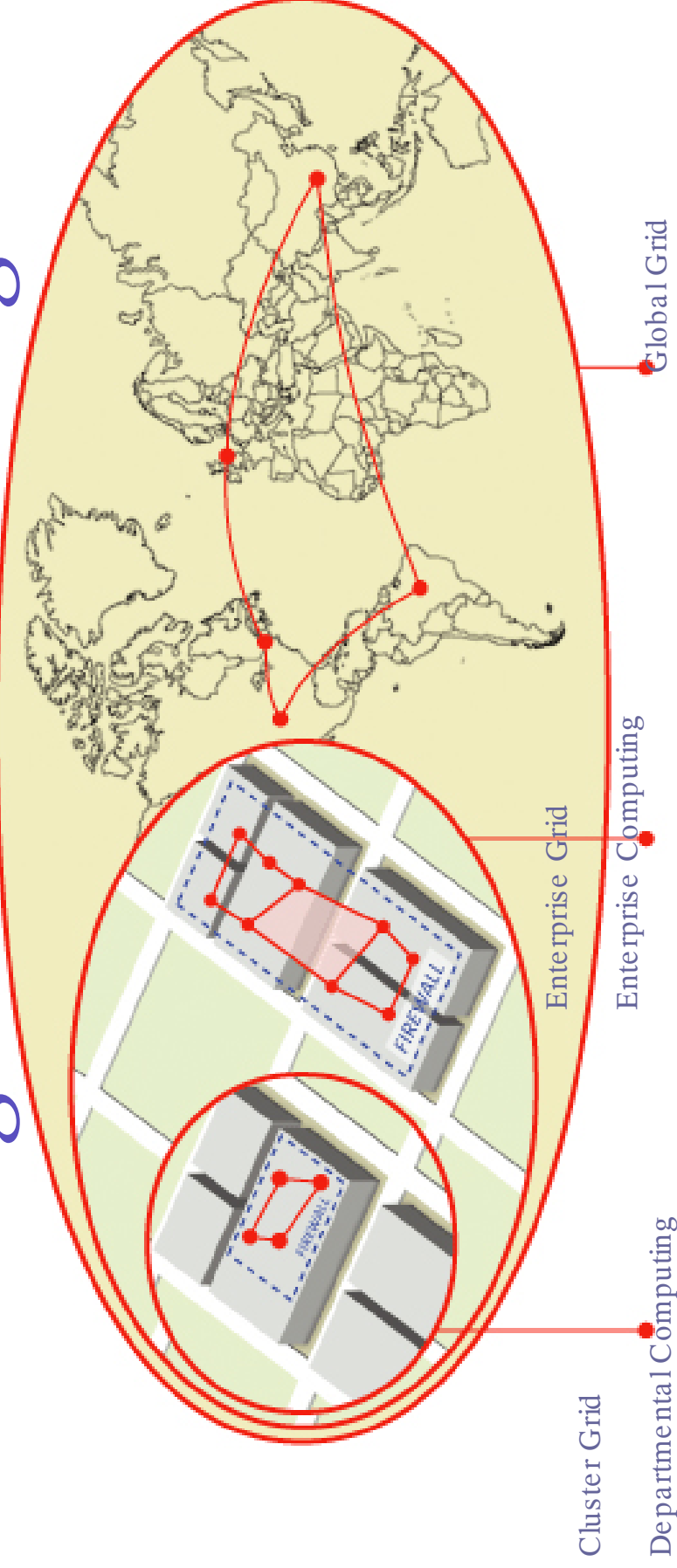
- **Data Distribution**
  - Location, volume, refresh, and security of data
- **Usability**
  - Skill set and client environment can impact usability of environment
  - Psychological factors important
- **Operations Management**
  - Limited staff to manage hundreds or thousands of CPUs
  - Resources added in large blocks
  - Change control is extremely critical operation

# Grid Engine

- Resource management software that aggregates compute power and delivers it as a network service.
- Provides consistent and pervasive access to high-throughput computational capabilities, and the job accounting and statistics needed to monitor and improve resource utilization.



# Grid Evolutionary Strategy: starting with the cluster grid

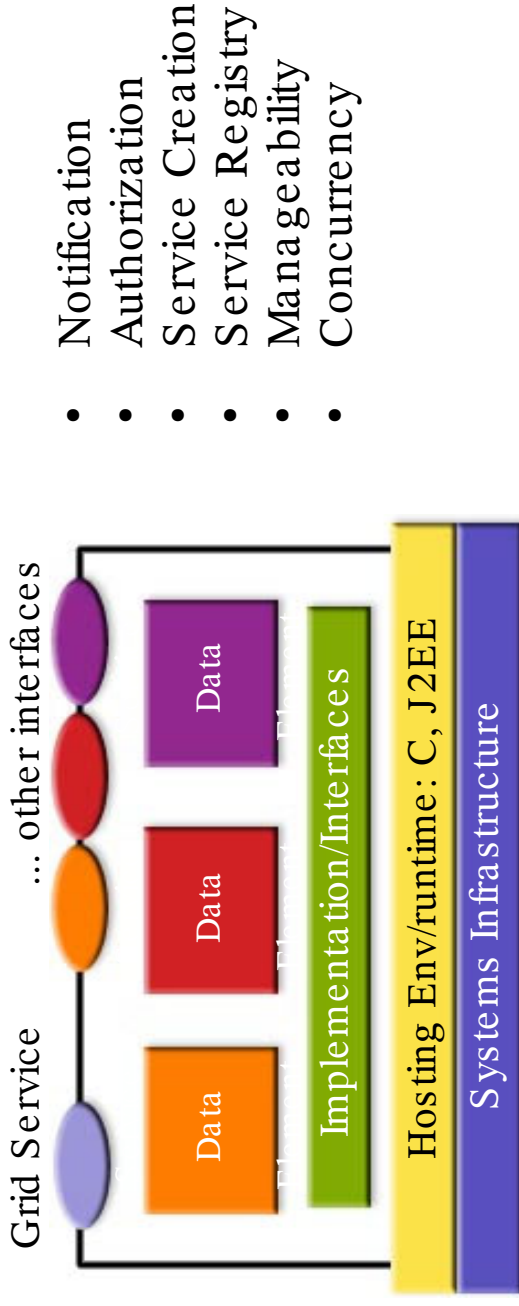


Internet Computing

- Simplest Grid deployment
- Maximum utilization of departmental resources
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- Policies ensure computing on demand
- Gives multiple groups seamless access to enterprise resources
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- Global view of distributed datasets

# Open Grid Services Architecture (OGSA)

- Evolution and Integration of Grid technologies and Web Services
- OGSA defines a “Grid Service”
- In terms of WSDL interfaces, defines mechanisms management systems
  - notification
  - lifetime management
  - change management



# Sun Collaborative

## Client Computing Portal

## Shared Pool of Resources

## Constituencies Sun Technologies

- Java™
- Jini™

- Sun ONE Studio™ Suite

### • Sun ONE™



- Java™
- Jini™

- Scientist
- Engineer

- Scientist developer
- Engineer developer
- Service Providers
- ISVs

- Virtualization of network, compute, storage resources—N1 initiative

- Resource optimization
- Thin-node and fat SMP clusters

- Single OS (m) scalability
- RAS

- Data Center managers
- IT stakeholders





# Usability

- Command line interaction to launch jobs
- GUI's often live in Unix® world
- Additional steps/products integrating with Windows OE
  - NFS Integration
  - Telnet windows
  - X Server
  - User ID Mgt.

- Technical Computing Portal

- Centralize Job Mgt.
- Standardize access and authentication
- Extend standard interface to users, customers, partners

## Technical Computing Portal powered by Sun Grid Engine


The screenshot displays the iPlanet Technical Computing Portal interface. At the top, a red banner features the iPlanet logo and the text "powered by Sun Grid Engine". Below this, a navigation bar includes links for "Home", "Options", "Content", "Layout", "Help", and "Log Out". The main content area is organized into several sections:

- User Information:** A "Welcome!" message for Frederic Partente, with a "Last Update:" timestamp of April 25, 2004 4:25:00 PM PDT and a "30 minutes max. life time" indicator.
- SunTCP Job List:** A section stating "You have no running jobs." with a "Submit new job..." link.
- Bookmarks:** A section with a "Enter URL Below:" input field and a "Sun home page" link.
- SunTCP Project List:** A list of projects including "Truck Benchmark", "Dummy project", "American option pricing", "Smith-Waterman genome blast", and "Ecoli blast", each with "edit" and "delete" links.
- SunTCP Application Portfolio:** A list of applications including "PAM-CRASH V2000D", "NCBI Blast 2.1.3", "Lassap 2.0", "American Put Option Pricer", "Sleepier demo application", and "Sleep Simulation".
- Applications:** A list of application types including "NetMail", "NetMail Lite", "NetFile", and "NetFile Lite".

The footer of the page contains the text "iPlanet Portal Server 3.0" and the same navigation links as the top bar.

# Sun Enabling Technologies

- Sun™ Grid Engine Software
  - High-throughput computational capabilities and resource utilization for cluster grids
  - Enterprise Edition adds policy management for shared-ownership campus grids
- Sun ONE™ Software
  - Portal Server: Internet services deployment platform
  - Services to quickly, securely deploy technically demanding portals

A yellow starburst graphic with multiple points, containing text.

Supports  
Solaris, Linux,  
and Other  
Operating  
Systems

# What is a Portal ?

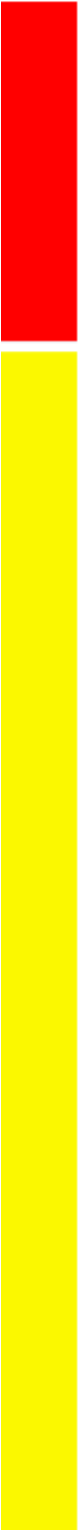
- A Web Server **plus**
  - Security
  - Authentication (Unix, LDAP, secured,...)
  - Personalization
  - Application Access (**business & technical**)
  - Content Aggregation

SunONE Portal Server<sup>©</sup>

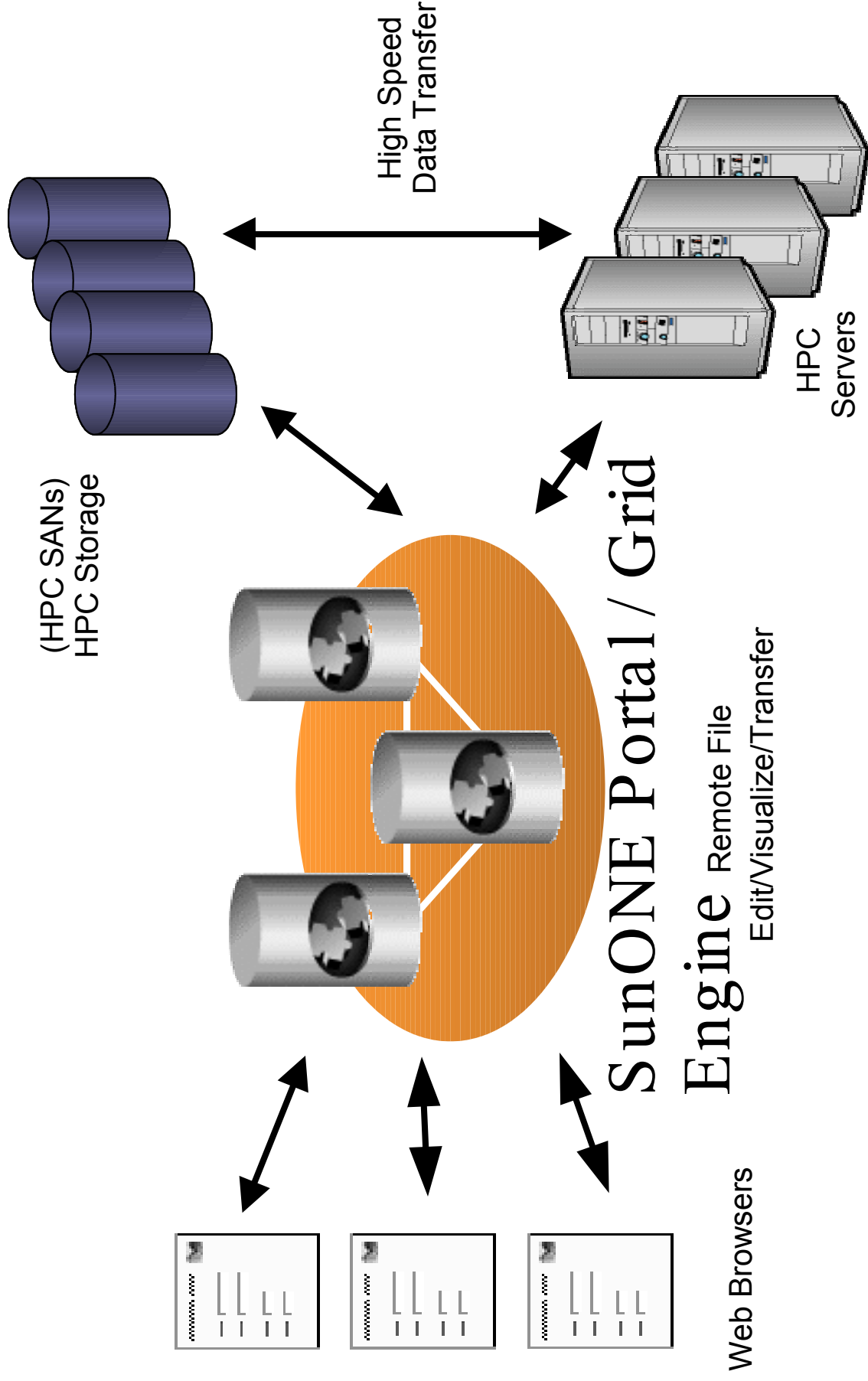
# What is an LS-DYNA Portal?

- LS-DYNA access through a Browser
  - Make system complexities *transparent*
  - Remote Access / Job Submission
  - Remote Job Management
  - HTML forms for job submission
  - Upload / Download files remotely
  - Separate Interfaces for Suppliers / Partners

**Secure anytime, anywhere access**



# LS-DYNA Portal Architecture



Web Browsers

SunONE Portal / Grid

Engine Remote File  
Edit/Visualize/Transfer

(HPC SANS)  
HPC Storage

High Speed  
Data Transfer

HPC  
Servers



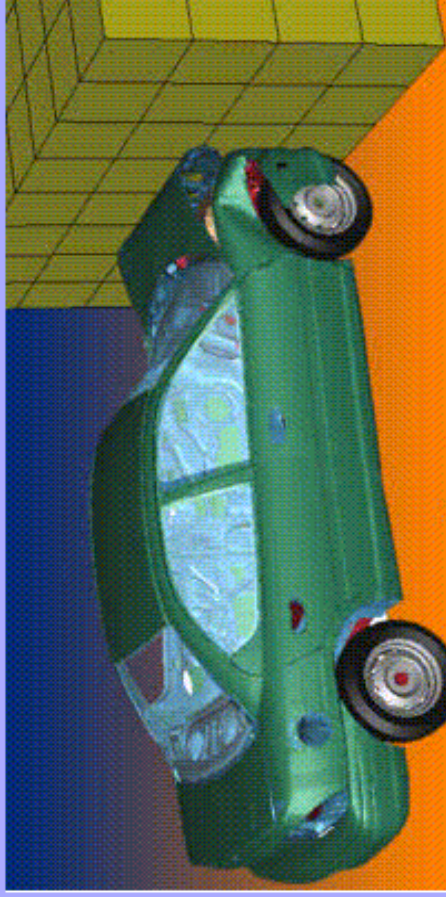
# Login Screen

**Technical Computing Portal**  
powered by Sun Grid Engine



A Sun | Netscape Alliance

This is a restricted access server



Unix User Password Login

Enter Your UserID

dyna1

Enter Your Password

\*\*\*\*\*

Submit



# User Access View

## Technical Computing Portal powered by Sun Grid Engine



### User Information

#### Welcome!

New User

Last Update:

March 27, 2002 9:51:47 AM PST

72 minutes left

30 minutes max idle time



### Job List

- Occupant S... [kill](#)

[Submit new job...](#)



### Netlet

No Netlet targets configured. Click "Edit" to configure Netlet targets.



### Bookmarks

Enter URL Below:

[Launch Xvnc server](#)

[Kill Xvnc server](#)



### Project List

- [Rigid Pole Crash Simulation: OpenMP 960](#) [edit](#) [delete](#)
- [Neon Frontal Crash Simulation: MPP 960](#) [edit](#) [delete](#)
- [Rigid Pole Crash Simulation: MPP 960](#) [edit](#) [delete](#)
- [Occupant Safety Simulation: OpenMP 960](#) [edit](#) [delete](#)

[Create new project...](#)



### Application List

- [LS-DYNA-MPP \(v.960\)](#)
- [LS-DYNA-SMP \(v.960\)](#)
- [Sleepier Demo Application](#)
- [SGE Qmon](#)



### Applications

[NetMail](#)

[NetMail Lite](#)

[NetFile](#)

[NetFile Lite](#)





# Job Submission

## SunTCP New Job Form

Project name: Rigid Pole Crash Simulation: MPP 960

Email notification:

Input arguments:

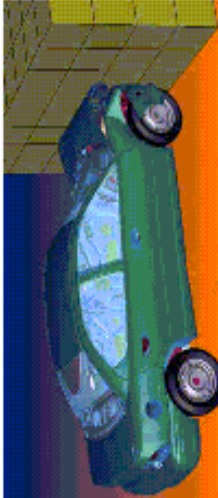
Output file name:

Error file name:

Number of CPUs:

# Job Input Form

Netscape:



## LS-DYNA-MPP Input Selection

Input Data :	<input type="text" value="Rigid Pole"/>
Run to ncycle :	<input type="text" value="1000"/>
Memory setting :	<input type="text" value="10000000"/>
Pfile name :	<input type="text" value="I"/>

[Help](#)

# File Viewer

## SunTCP Project Information

Project name: Rigid Pole Crash Simulation: OpenMP 960

Application: SMPDYNAFORM

Exports:

Files: [.suntcp-project](#)

[.suntcp-su](#)

[rp200p2.out](#)

[rp200p2.err](#)

[messag](#)

[d3hsp](#)

[d3plot](#)

[d3thdt](#)

[status.out](#)

[d3dump01](#)

[d3plot01](#)

[d3thdt01](#)

[head](#)

[tail](#)

[head](#)

[tail](#)

[head](#)

[tail](#)

[head](#)

[tail](#)

[head](#)

[tail](#)

[head](#)

[tail](#)

Continue

# Output File

## SunTCP File View

estimated clock time to complete = 12399 sec ( 3 hrs 26 mins)

```
1 t 0.0000E+00 dt 1.16E-06 flush i/o buffers
1 t 0.0000E+00 dt 1.16E-06 write d3plot file
```

\*\*\*\*\* termination cycle reached \*\*\*\*\*

```
200 t 2.3176E-04 dt 1.16E-06 write d3dump01 file
200 t 2.3176E-04 dt 1.16E-06 write d3plot file
```

N o r m a l t e r m i n a t i o n

Storage required for explicit solution: 1067632

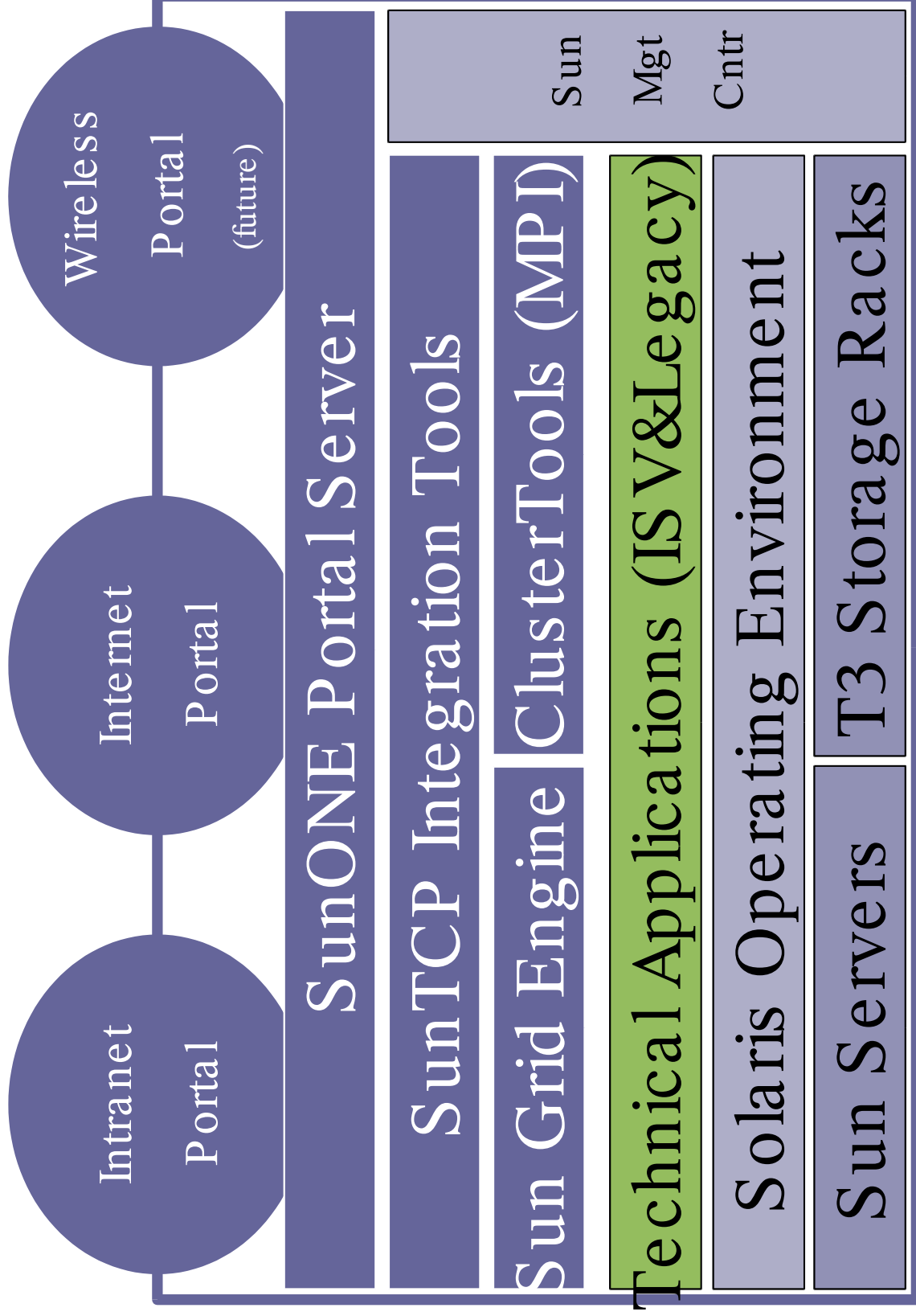
T i m i n g	i n f o r m a t i o n	%CPU	Clock(seconds)	%Clock
-----	-----	-----	-----	-----
Initialization	1.7300E+00	4.26	9.0089E-01	4.42
Element processing	3.6780E+01	90.52	1.8315E+01	89.91
Binary databases	1.7000E-01	0.42	8.8151E-02	0.43
ASCII database	0.0000E+00	0.00	1.4046E-03	0.01
Contact algorithm	1.9500E+00	4.80	1.0620E+00	5.21
Interface ID	1 1.9200E+00	4.73	1.0542E+00	5.18
Contact entities	0.0000E+00	0.00	0.0000E+00	0.00
Rigid bodies	0.0000E+00	0.00	3.2400E-03	0.02
Implicit Nonlinear	0.0000E+00	0.00	0.0000E+00	0.00
Implicit Lin. Alg.	0.0000E+00	0.00	0.0000E+00	0.00
-----	-----	-----	-----	-----
T o t a l s	4.0630E+01	100.00	2.0370E+01	100.00

```
Problem time = 2.3176E-04
Problem cycle = 200
Total CPU time = 41 seconds ( 0 hours 0 minutes 41 seconds)
CPU time per zone cycle = 35635 nanoseconds
Clock time per zone cycle = 17835 nanoseconds
```

```
Number of CPU's 2
Start time 03/27/2002 10:18:48
End time 03/27/2002 10:19:10
Elapsed time 22 seconds ( 0 hours 0 minutes 22 seconds)
```



# TCP Hardware and Software Stack



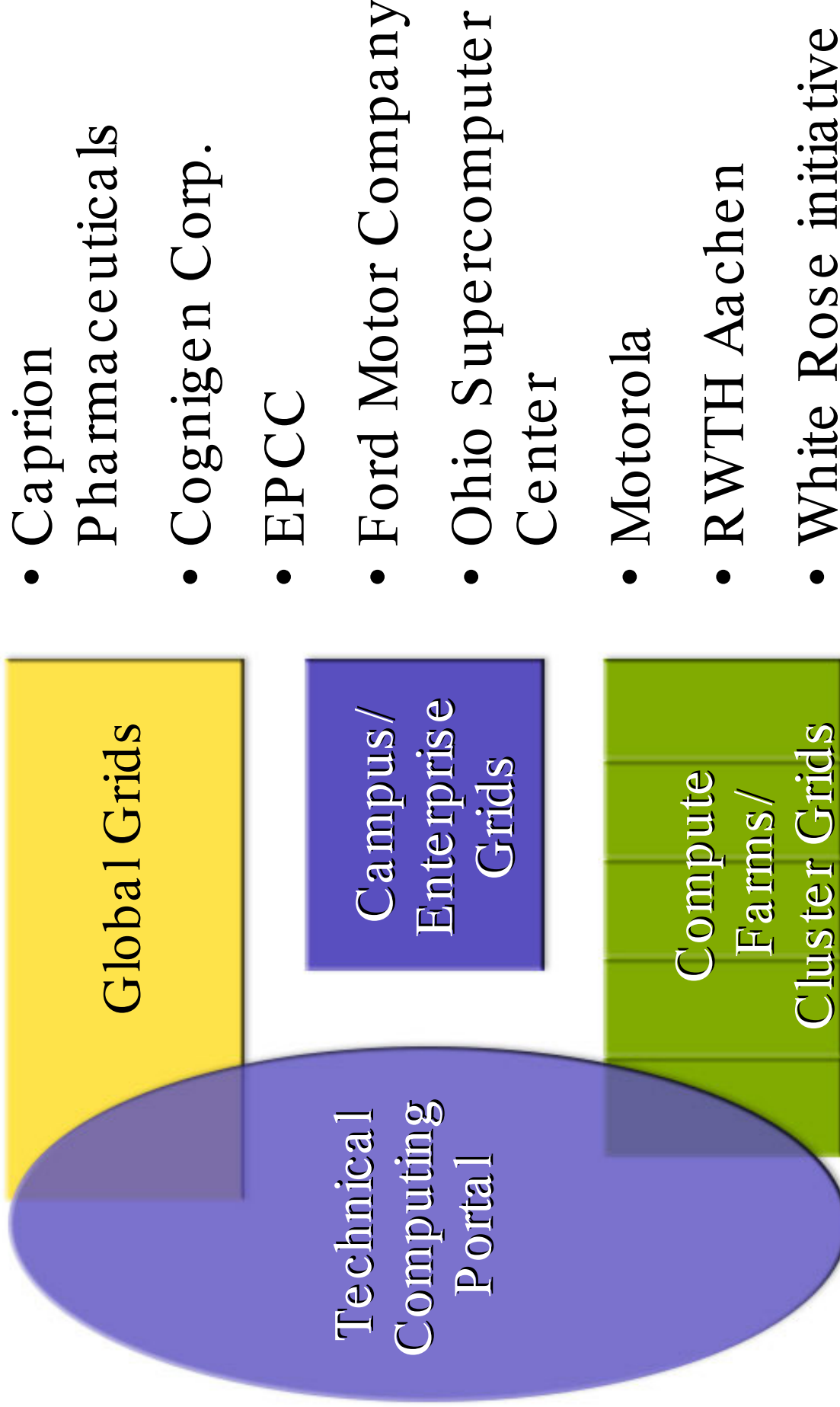


# With TCP, You Can...

- Enjoy secure *anytime, anywhere access* – submit jobs remotely
- Make HPTC resources available to other users without duplicating the investment
- Upload files with the click of a button
- Improve resource management and harness idle computing cycles
- Manage job submission via forms
- Dynamically check on the status of jobs
- Receive email notification when jobs are complete
- Download/visualize output files remotely
- Easily share results with collaborators
- Quickly add legacy apps for sharing and remote use



# Sun Powers the Grid



# Ford Motor Company



- **Sun HPTC solution**
  - 500 dual-CPU workstations
  - Sun Grid Engine software
- **Business Impact**
  - Run MCAD applications on 500 CPUs by day
  - Run MCAE applications 7 x 24 on same systems configured as a grid
    - 500 CPUs daytime; 1000 CPUs nights and weekends
  - Greatly increased throughput
  - More analysis drives higher quality research and lower cost
  - Faster design decisions reduce time to market

# Caprion Pharmaceuticals:

## LEADING PROTEIN ANALYSIS COMPUTE FARM

- Sun HPTC solution

- Based on SPARC/Solaris
- Range of Sun Fire servers (280R to 6800)
- Forte™ (Sun Studio) Development Tools
- Sun Professional Services



- Bioinformatics firm, leader in proteomics

- Discovers and develops pharmaceutical products

- Criteria

- Build compute farm that can address the biggest issues in life sciences today
- Process hundreds of terabytes of data per year
- Create architecture that can grow exponentially
- Better collaboration, faster time-to-market

# Aachen University

- **Leading European technical university**
  - Replace outdated, vector-based supercomputer
  - Four teraflops goal
  - Collaboration focus on CFD and VR Tools
- **Criteria**
  - ISV relationships
  - Scalability, availability
  - Price/performance
  - Vendor with collaboration-oriented approach



**RWTHAACHEN**

- **Sun HPTC solution**
  - Four Sun Fire 15K systems, 16 Sun Fire 6800 systems
  - Aggregates to 1.2 teraflops
  - Sun™ HPC ClusterTools software
  - Sun™ Grid Engine for statewide access

# HPC Virtual Labs (HPCVL)

- Consortium of Four Canadian Universities
  - Recently deployed massive Sun HPC environment
  - Expected to be among top 100 HPC sites in the world
- Criteria
  - Innovative partnership program
  - Robustness, reliability
  - Price/performance
  - Future product roadmap
- Sun HPTC Solution



- 10 Sun Fire™ 6800s and 2 Sun Fire 15Ks
- Sun Enterprise™ 220R, Sun StorEdge™ T3 arrays
- Solaris™ 8 Operating Environment
- Sun HPC ClusterTools™, Forte™, Sun Grid Engine, Sun Resource Manager™, Sun Management Center, Solstice DiskSuite™ software

# Conclusions

Grid Computing has the potential to extend computing into a utility-type environment. If this is to happen, Grid computing must be built upon an infrastructure designed to provide carrier-grade Quality of Service