

Sun-APSTC Initiative in Asia Pacific

Dr Simon See

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High Performance Computing Technology

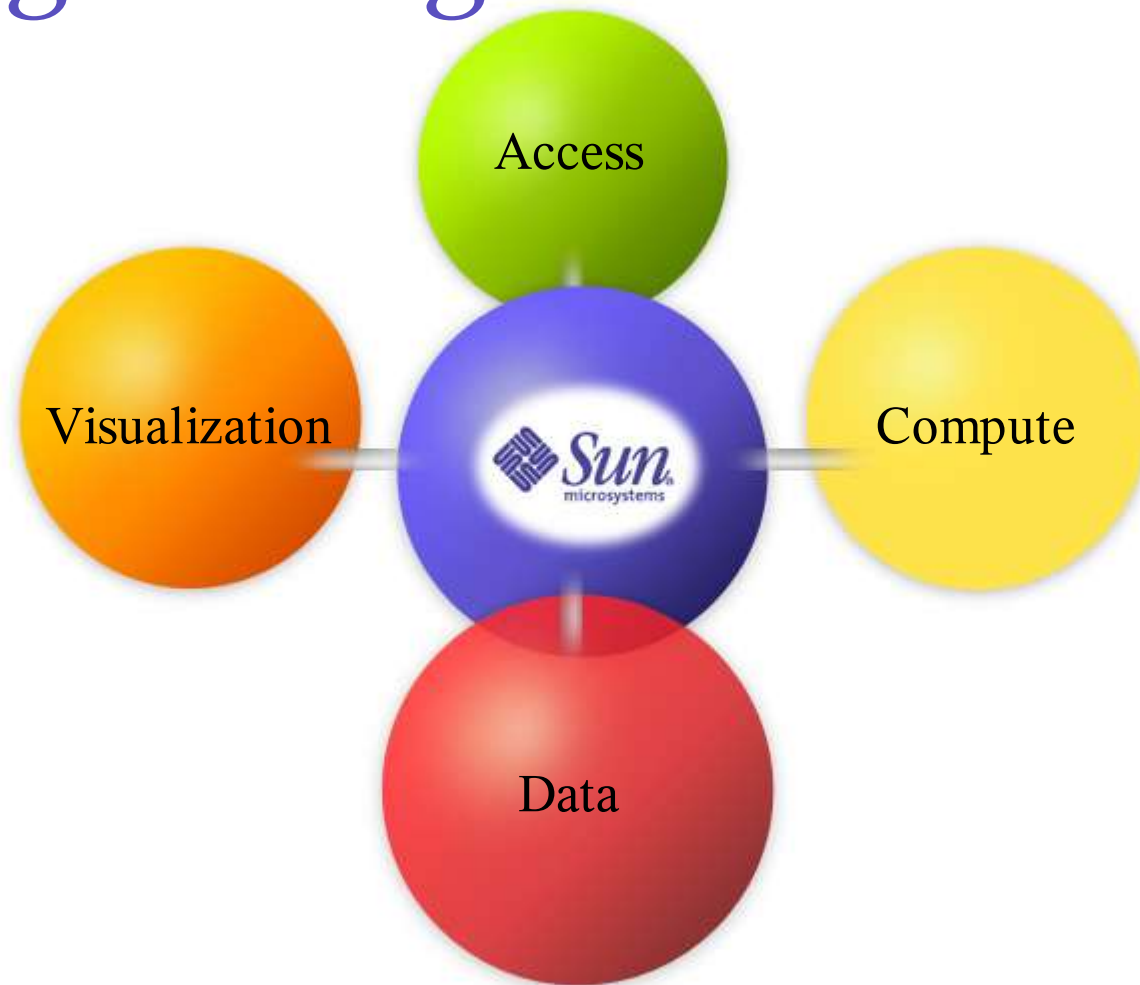
Asia Pacific Science and Technology Center

and

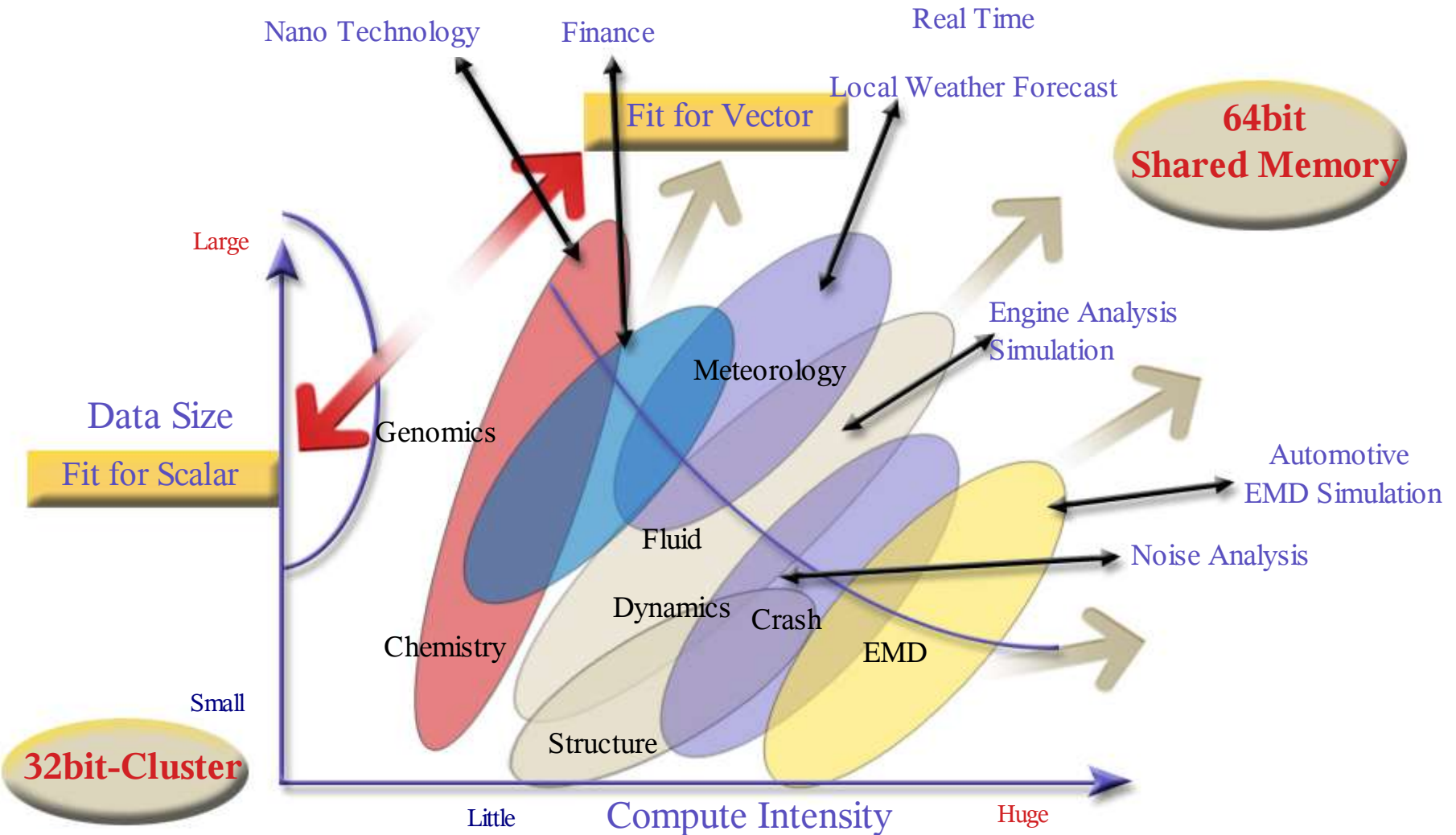
Associate Professor

Nanyang Technology University

Key Scientific and Engineering Functions

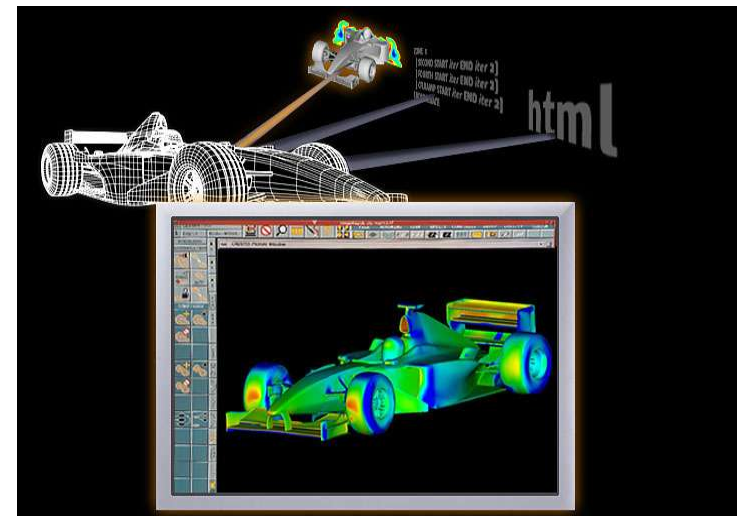


Vertical vs. Horizontal Workloads

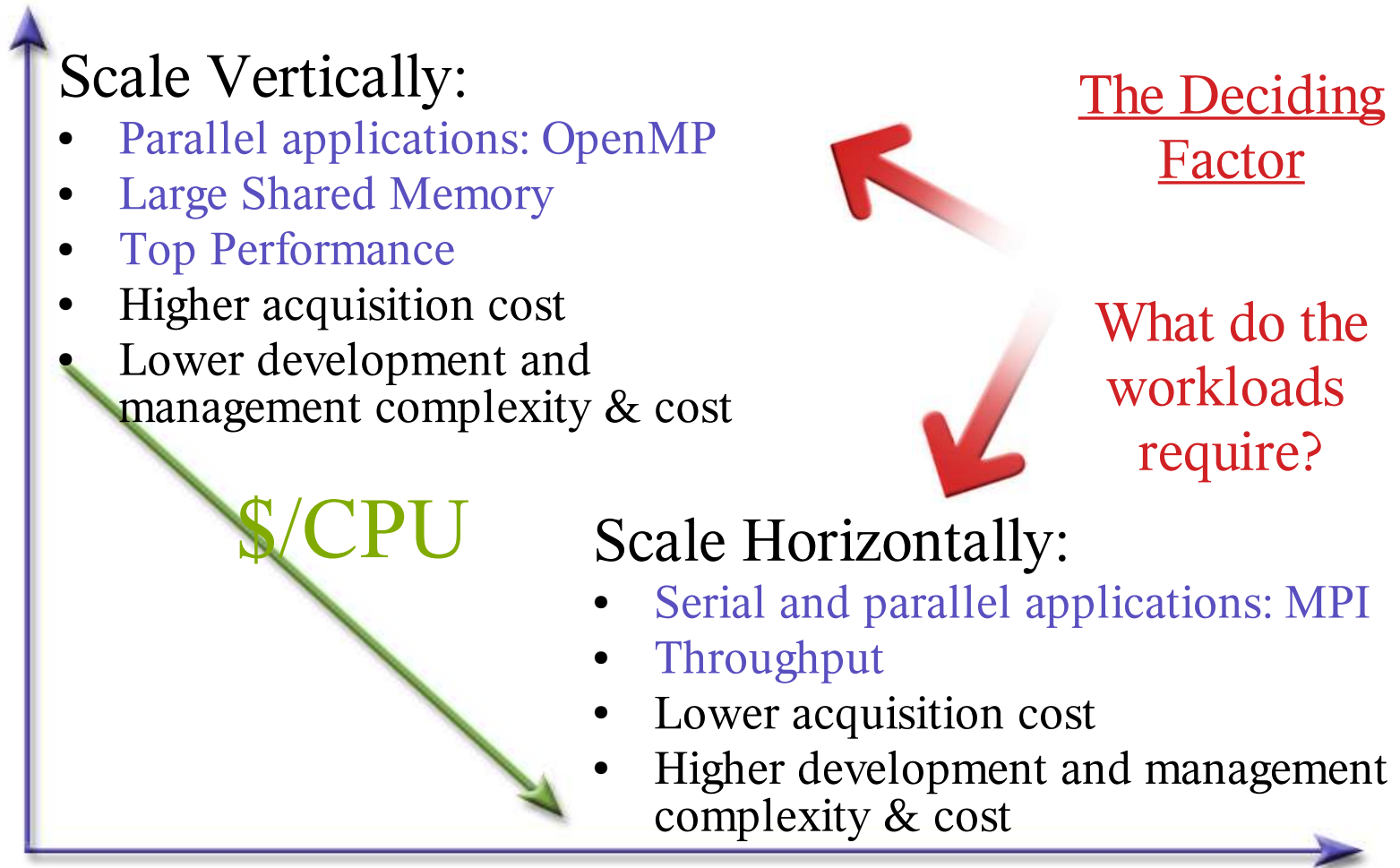


IT Requirements for HPTC

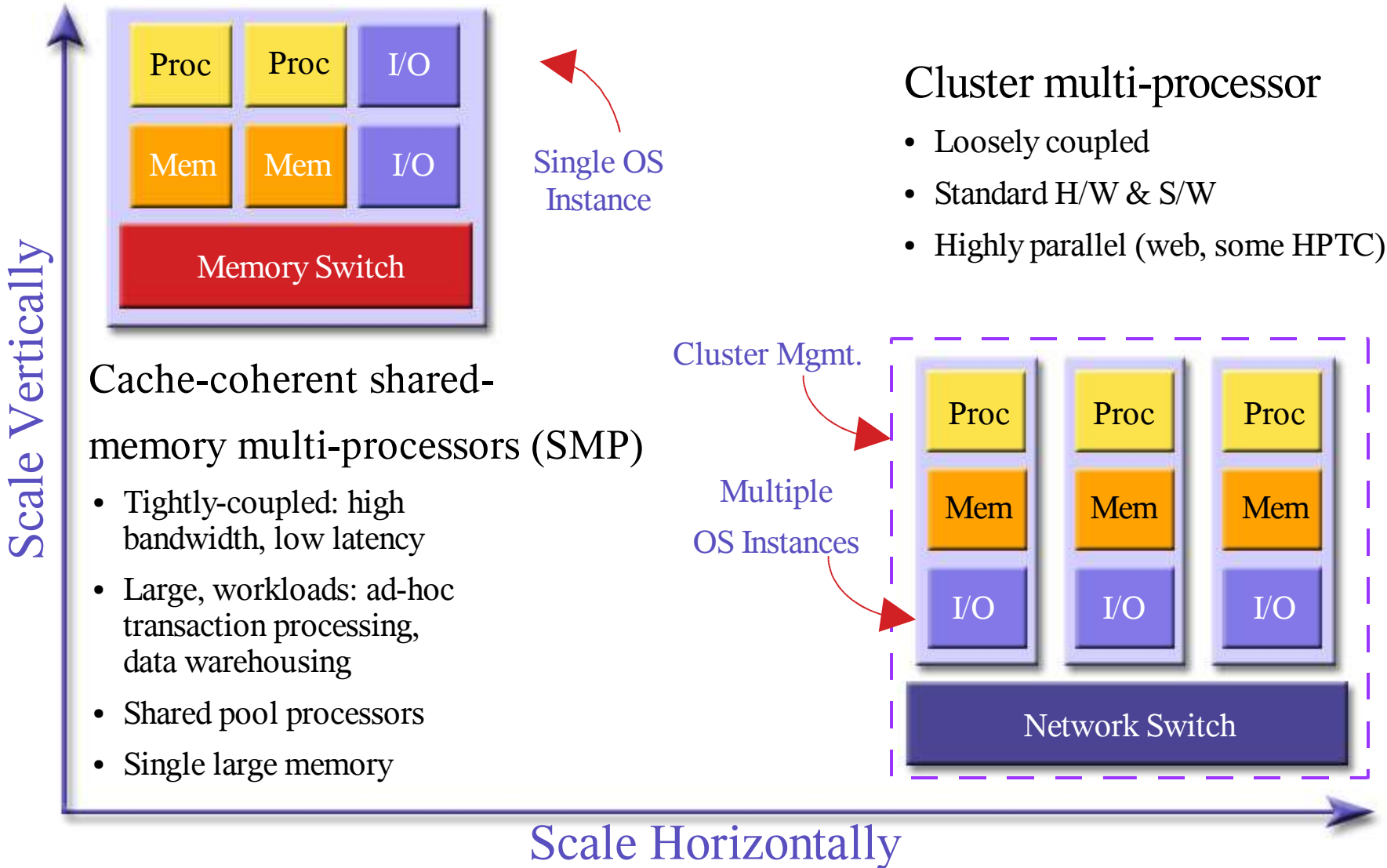
- NO single platform or architecture is best fit for ALL type of applications



The HPTC Architecture Dilemma: Scale Vertically or Scale Horizontally?



Scale Vertically or Horizontally



Vertical vs. Horizontal Workloads


Scale Vertically

- Commercial Workloads
 - Large databases
 - Transactional databases
 - Data warehouses
- HPTC Workloads
 - Climate modeling
 - Data mining
 - Signal Processing
 - Cryptanalysis
 - Nuclear simulation
 - Some structural analysis
 - EDA full assembly simulation

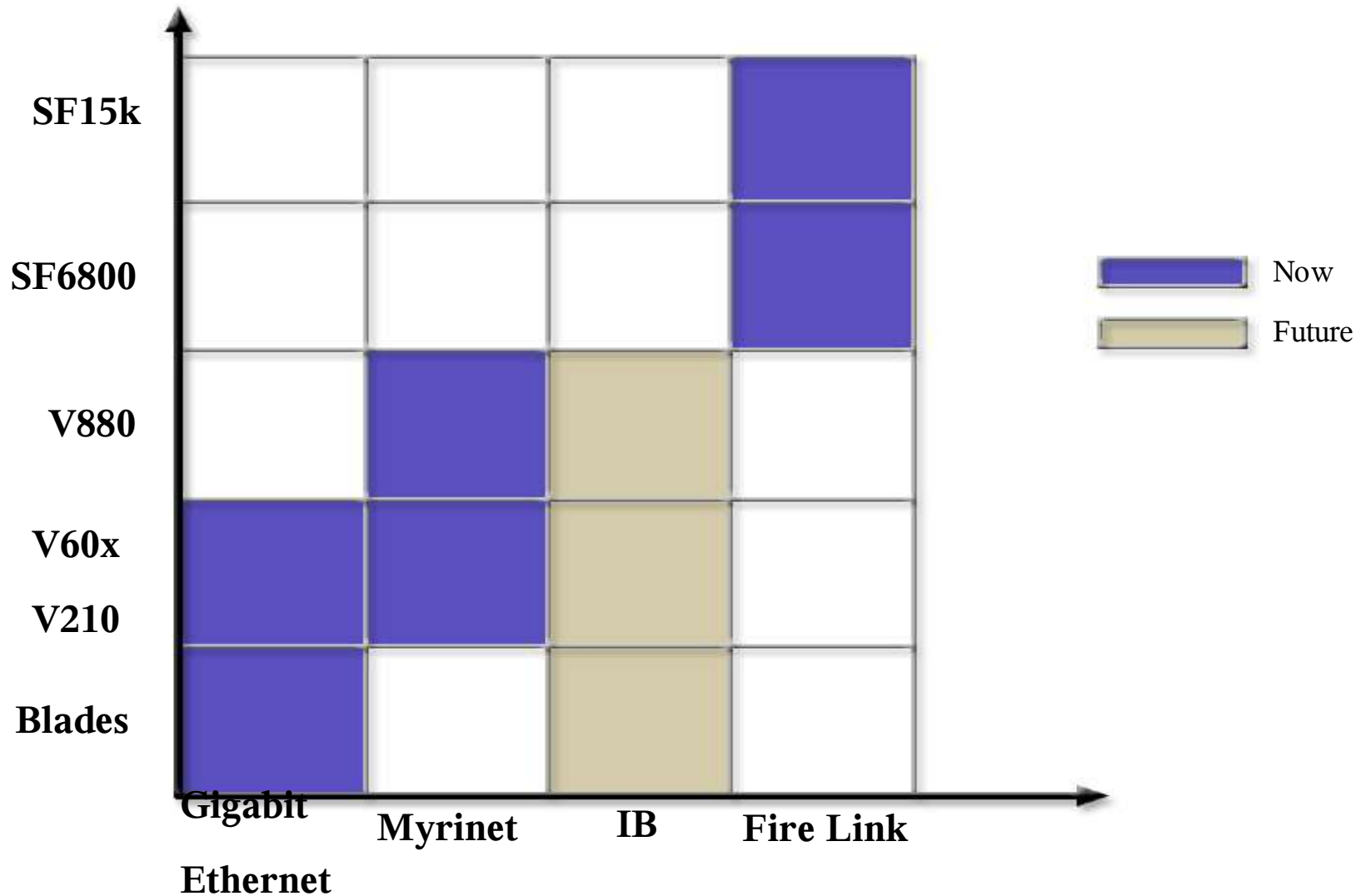
Scale Horizontally

- Commercial Workloads
 - Web servers, Firewalls
 - Proxy servers, Directories
 - SSL, VPN
 - Media streaming
 - XML processing
- HPTC Workloads
 - Seismic analysis
 - Genomics
 - Computational Fluid Dynamics
 - EDA sub-assembly simulation
 - Some Structural Analysis
 - Crash Testing

Workload Performance Factors

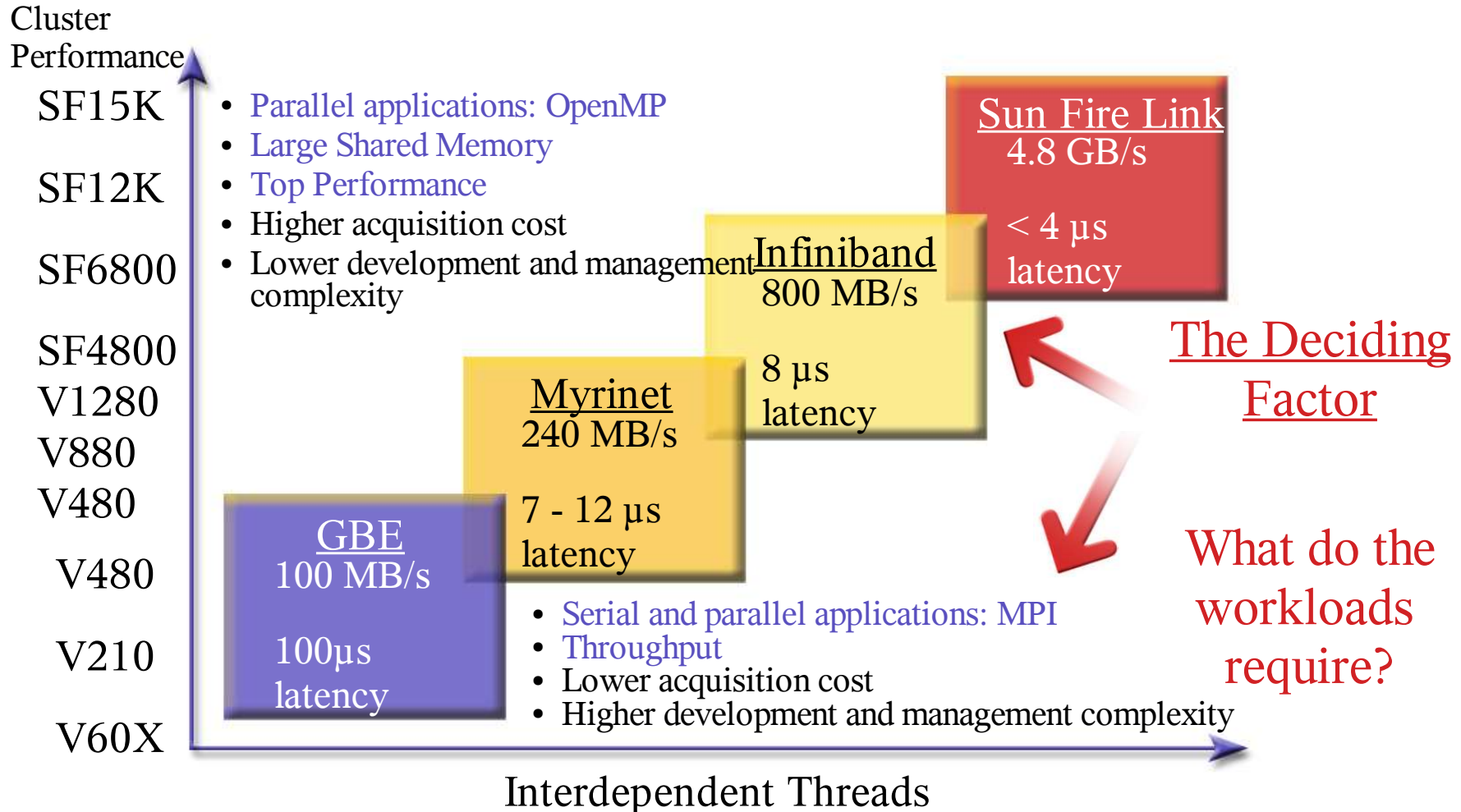
- Processor speed, capacity and throughput
 - Memory capacity
 - **System interconnect latency & bandwidth** 
 - Network and storage I/O
 - Operating system scalability
 - Visualization performance and quality
 - Optimized applications
 - Network service availability
- #1 issue
for real world
cluster
performance
and scaling

Compute Grid Family



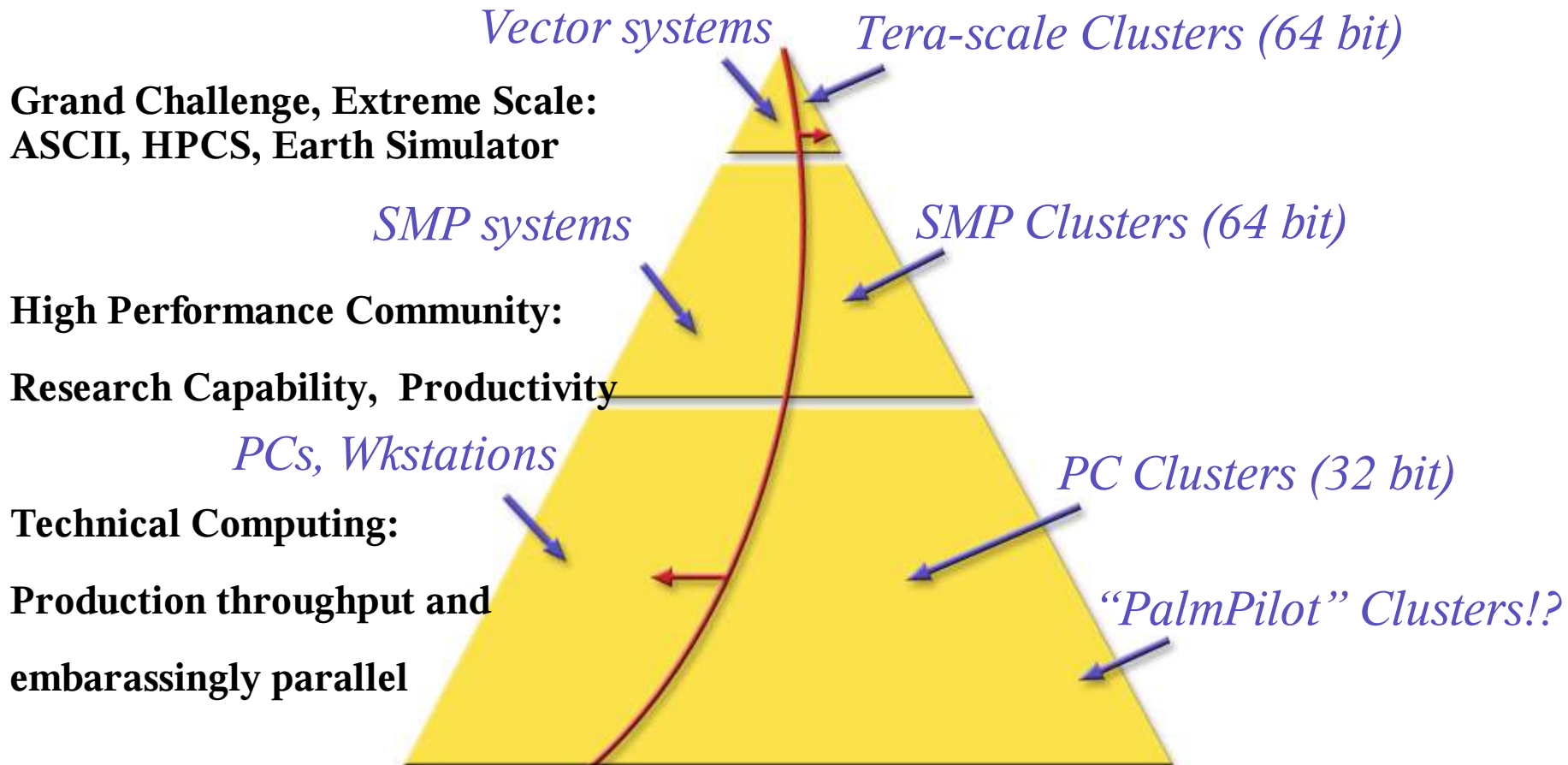
Interconnect Options

Scale Vertically or Scale Horizontally?



HPTC Market:

Moving to Clusters



Market Trends & Business

Climate

- Shift from performance to productivity
- Market shifted to SMPs and now shifting increasingly to clusters
- Proliferation of “industry standard” systems
- Research market often procuring to peak Teraflops (which drives toward commodity)
- Increasing influence of IT over engineering & research end-users (drives toward commodity)
- Linux frequently written into procurements
- Buying cycles stretching due to budget environment and accountability

HPTC: Critical Business Needs

Effectiveness

Make the right choice between capability and cost!

- Scalable, heterogeneous, distributed data access
- Scalable end-to-end computing architectures
- Simplified application development and deployment
- Simplified system management and delivery of services
- Scalable and distributed visualization

Provide the required services at an acceptable cost

Cost and
Complexity

The Network is the Computer

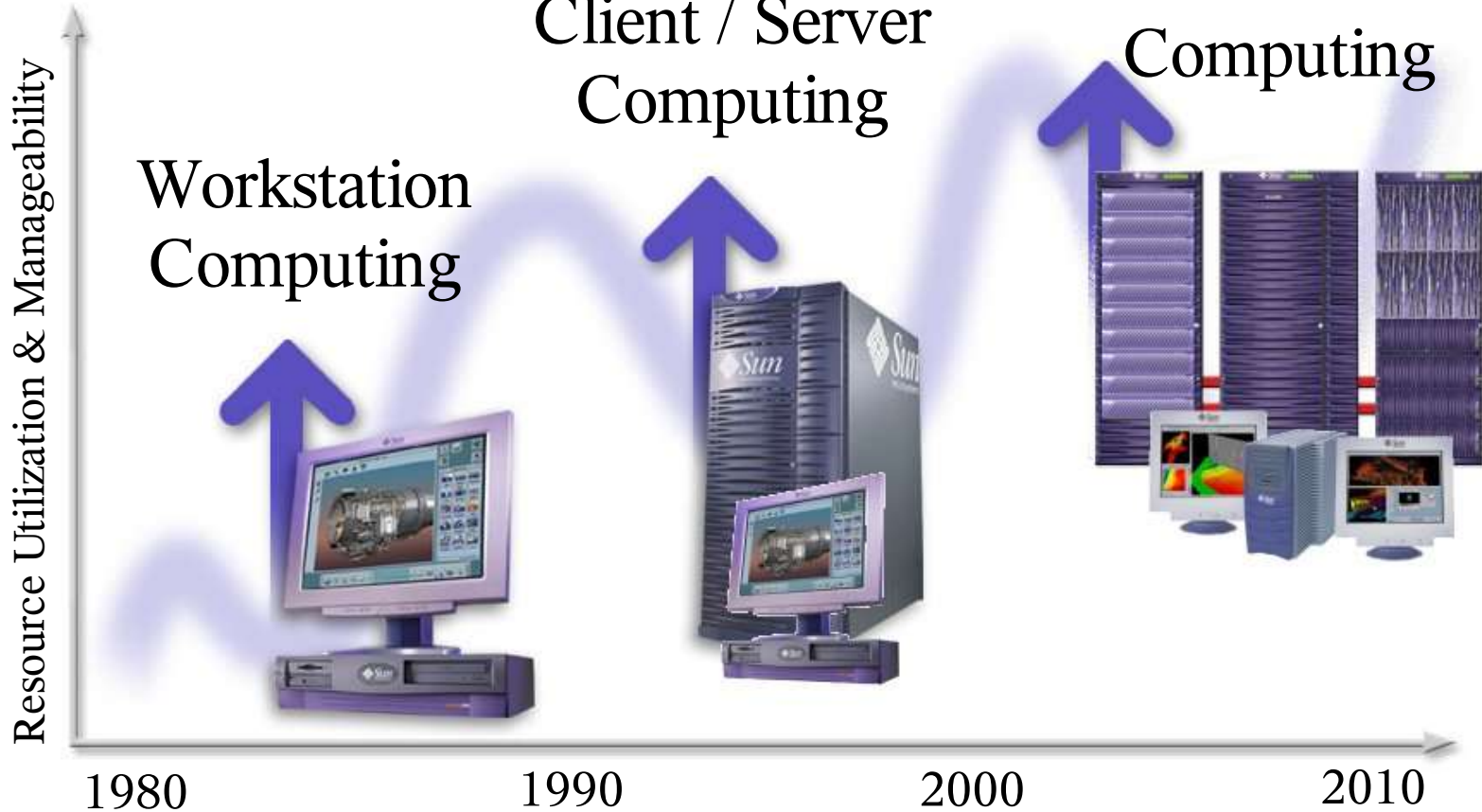
Evolution in HPTC

GRID

Computing

Client / Server
Computing

Workstation
Computing



GRID as an Operational Concept

Workflow Service Definition & Mapping

Capability Computing Services

Data Storage,
Management
and Access
Services

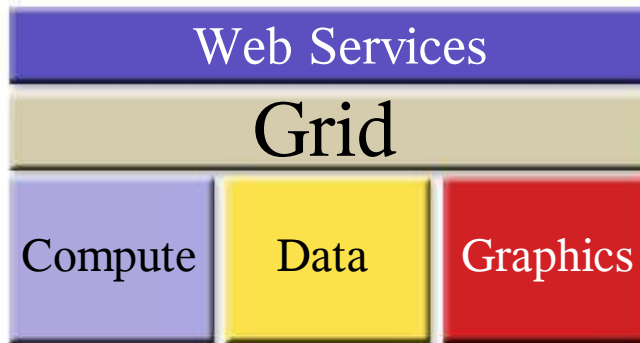


Capacity
Computing
Services



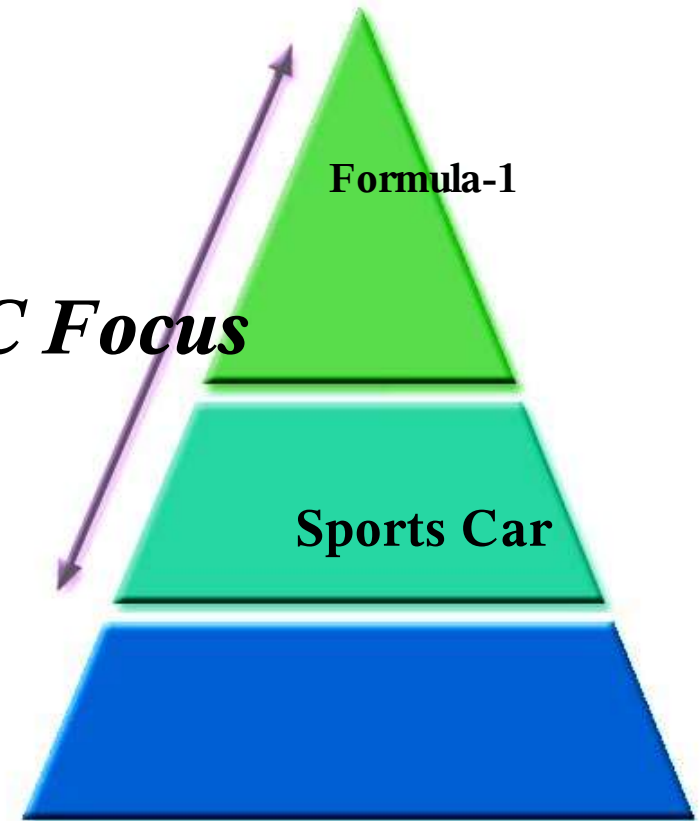
Collaboration,
Graphics,
and
Visualization
Services

HPTC Strategy

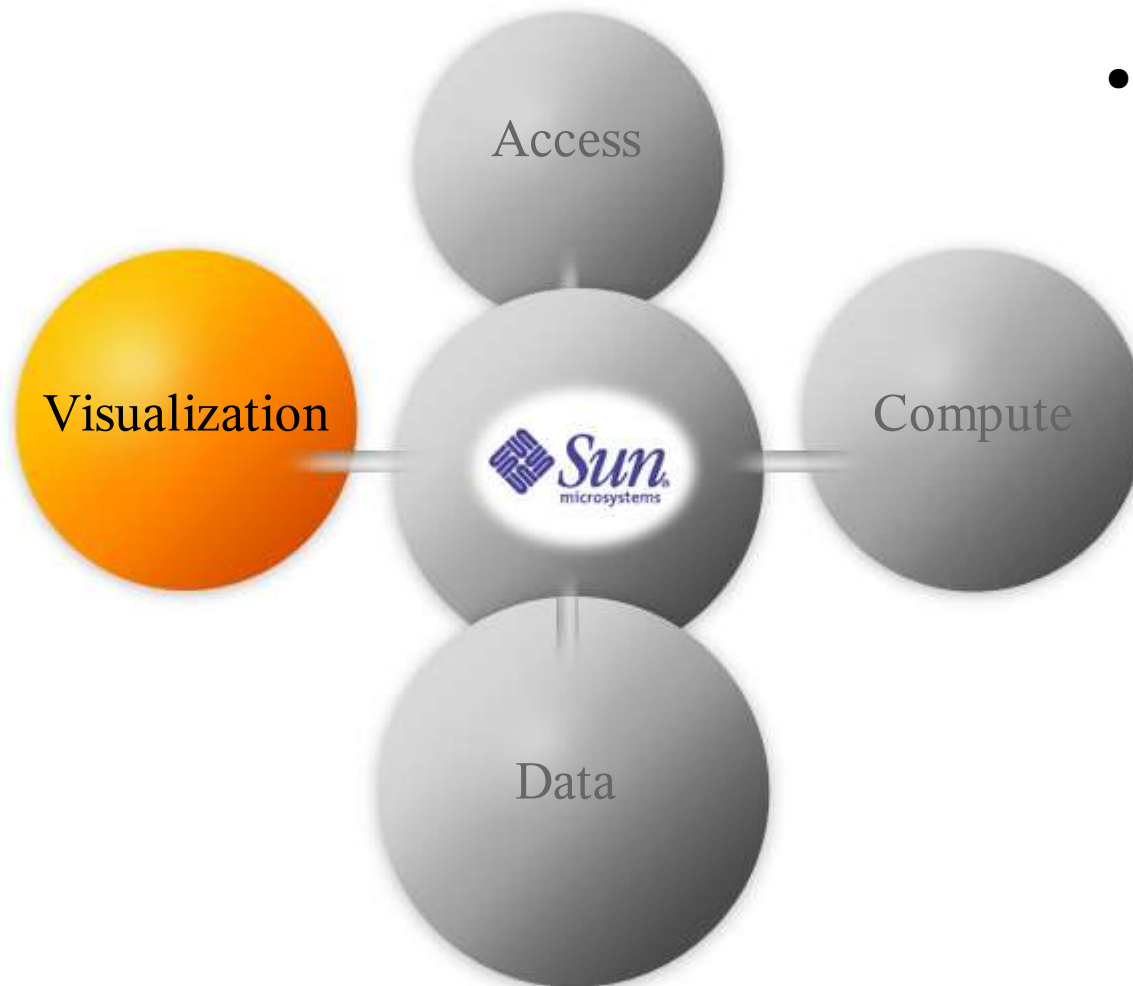
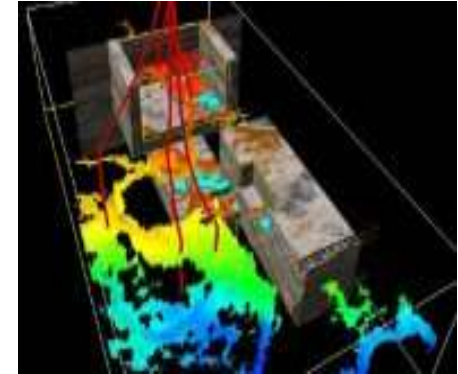


- **Industry Trend: Grid**
 - “All Grid, All the Time”
 - Grid product family
- **Seeds: High-End**
 - HPCS, iHEC
 - Sun Labs interface
- **GTM: Solutions**
 - Intersection of “solutions” and Grid
- **Technology: HPTC Web Services**
 - GGF, OGSA, select ISVs, Web Svcs

HPTC Focus



Key Scientific and Engineering Functions



- Needs

- Interactive visualization of extremely large data sets
- Ability to view data in large-screen collaborative, immersive environment
- Performance scalability
- Visual quality
- Ease of application deployment in multi-display environments

Graphics Grid:

Access for More Users to Visualization Services at Required Visual Quality and Performance Levels

Storage



SAN/
NAS

Compute



Compute Cluster

Graphics
InterConnect

Visualization



• Digital

• Video

• Delivery

Visualization

Services

Over

LAN/WAN

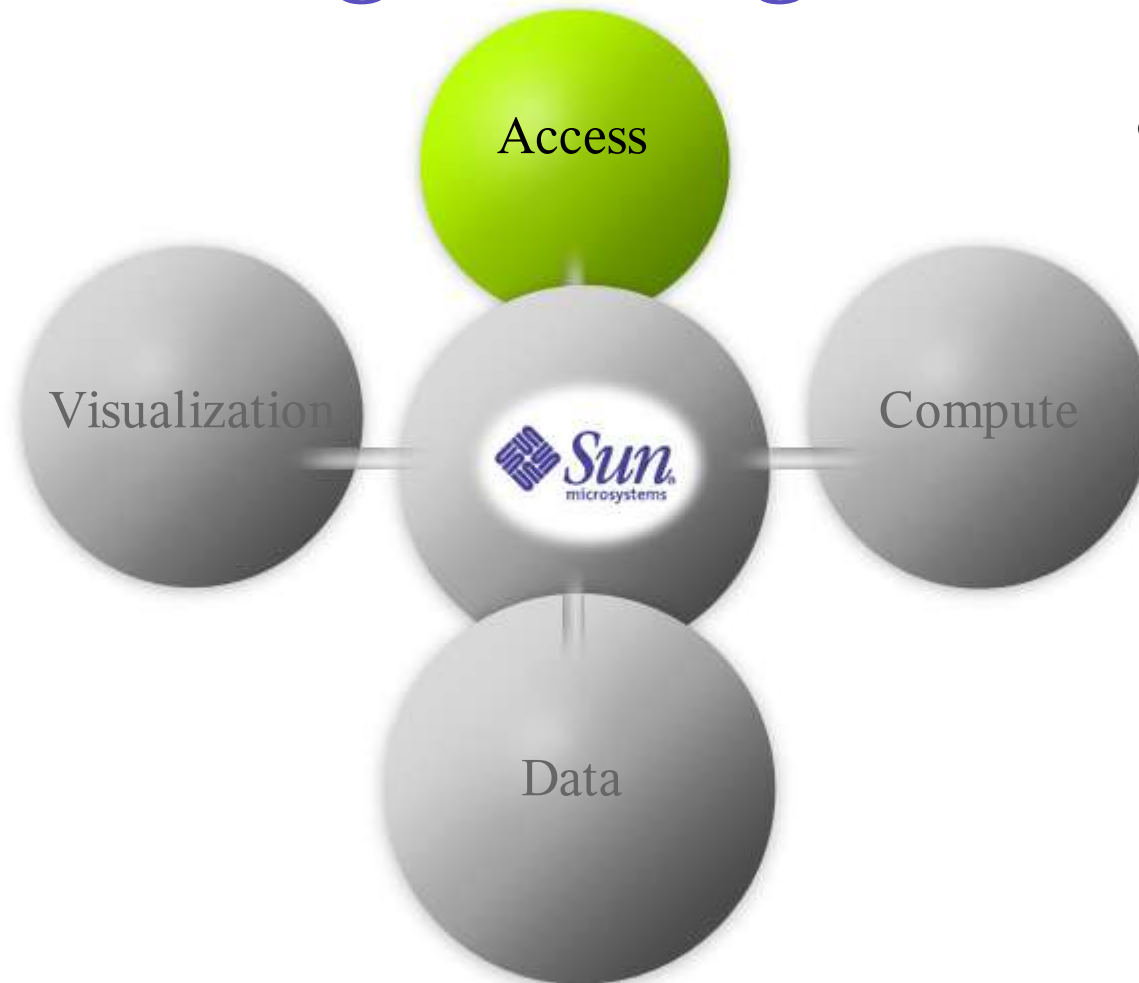


Display



Clients

Key Scientific and Engineering Functions



- Needs
 - Improve user access experience
 - Sharing resources
 - Simplify delivery of technical apps and services
 - Collaborative development environment

Sun Collaborative Computing

Client

- Java™
- Jini™
- Java™
- Jini™
- Scientist
- Engineer

Portal

- Sun ONE Studio™ Suite
 - Sun ONE™
- 
- Scientist developer
 - Engineer developer
 - Service Providers
 - ISVs

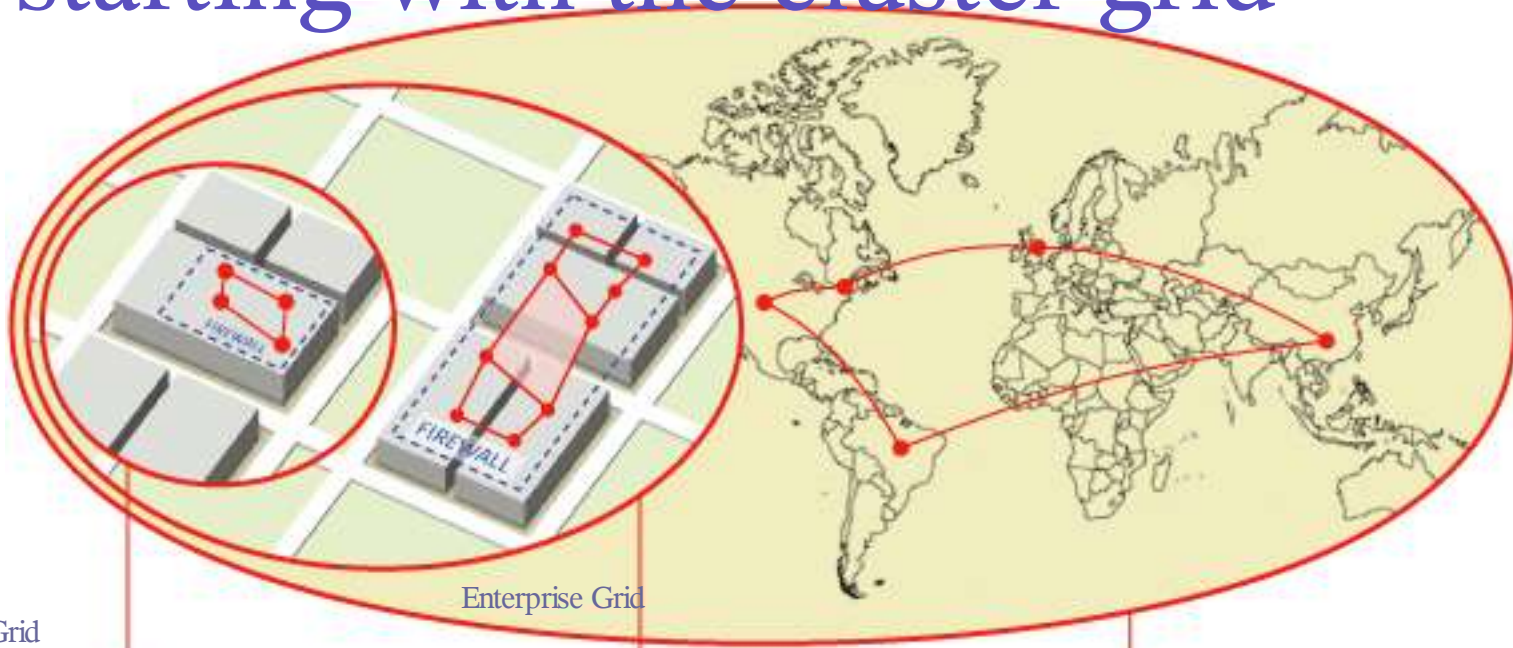
Shared Pool of Resources

- Virtualization of network, compute, storage resources—N1 initiative
- Resource optimization
- Thin-node and fat SMP clusters
- Single OS (monolithic) scalability
- RAS
- Data Center managers
- IT stakeholders



Constituencies Sun Technologies

Grid Evolutionary Strategy: starting with the cluster grid



Cluster Grid

Departmental Computing

Enterprise Grid

Enterprise Computing

Global Grid

Internet Computing

- Simplest Grid deployment

- Maximum utilization of departmental resources

- 21 • Resources allocated based on

- Resources shared within the enterprise

- Policies ensure computing on demand

- Gives multiple groups seamless

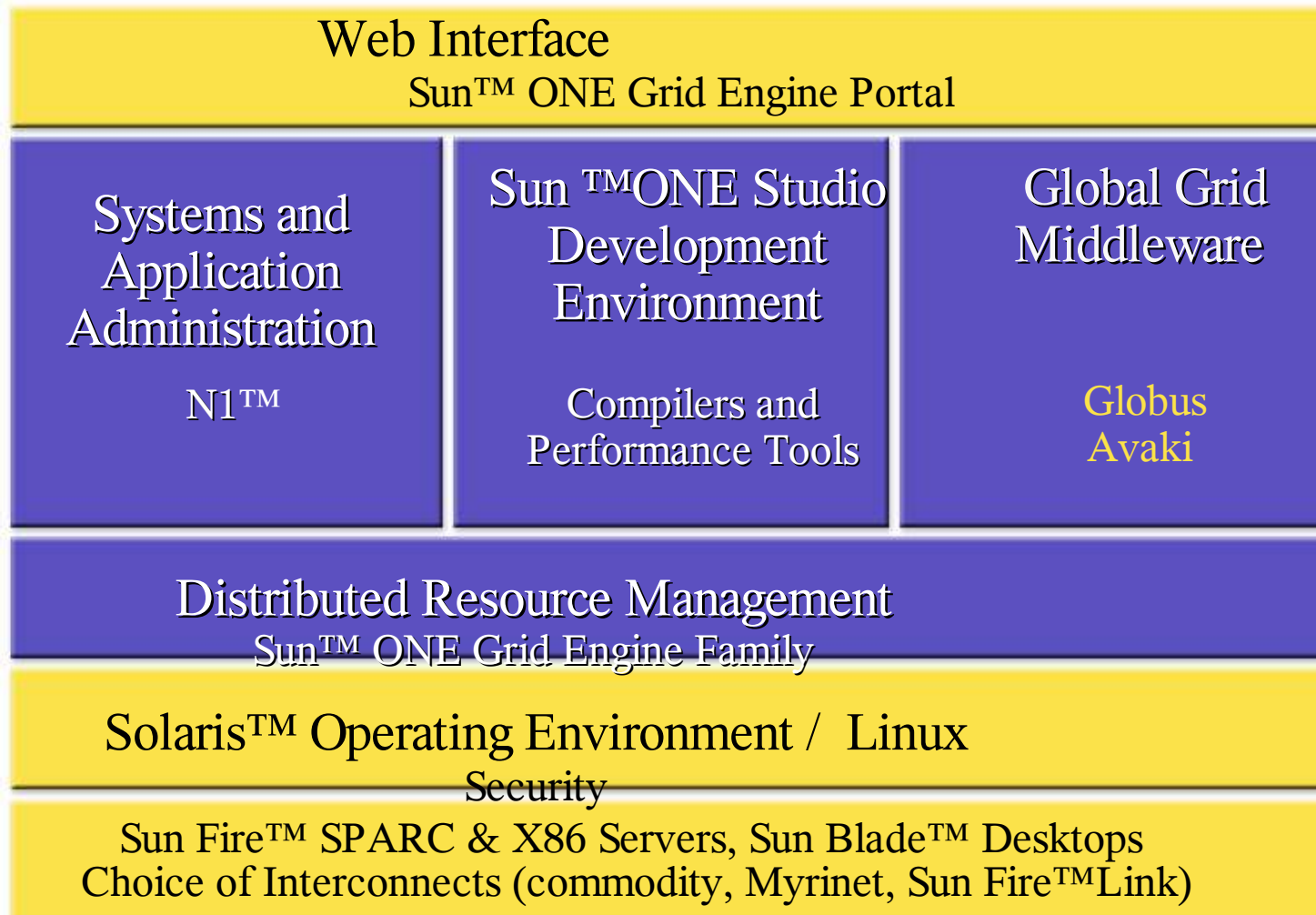
- Resources shared over the Internet

- Global view of distributed datasets

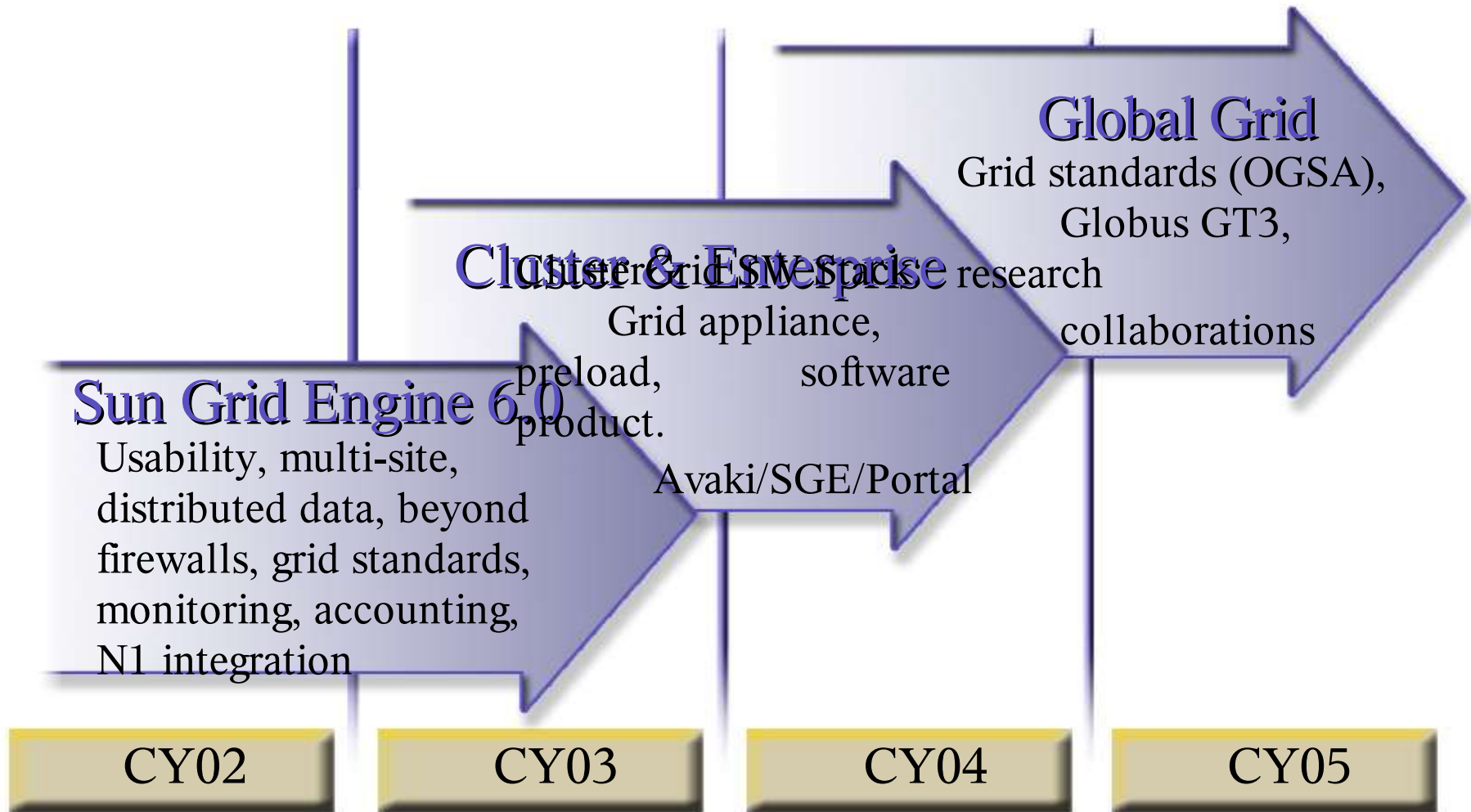
- Growth path for enterprise Grids

Grid Infrastructure Software:

Integrated Stack

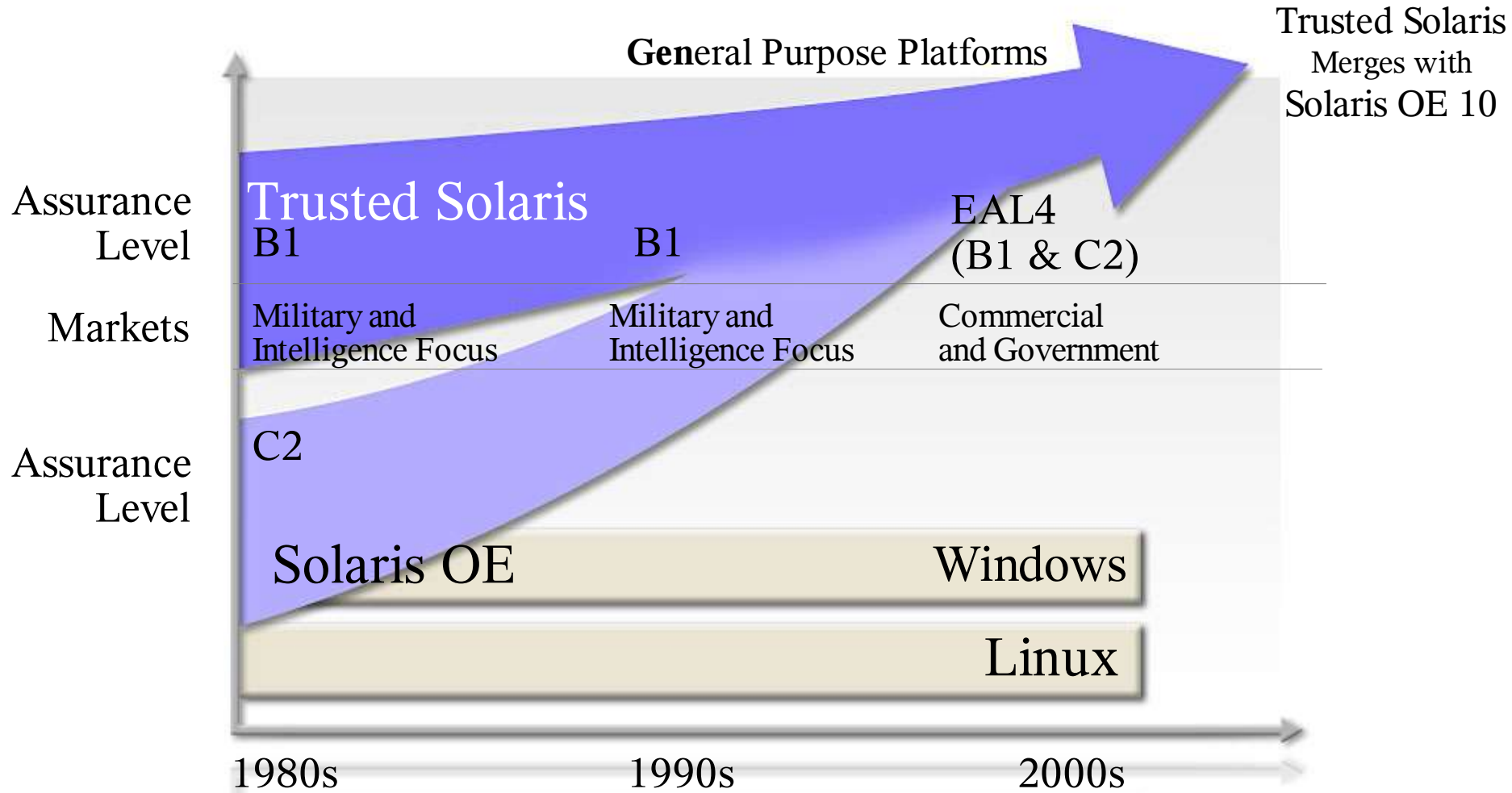


Sun Grid Products Roadmap




One Secure Solaris OE

Government Level Security for 32- and 64-bit Platforms



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

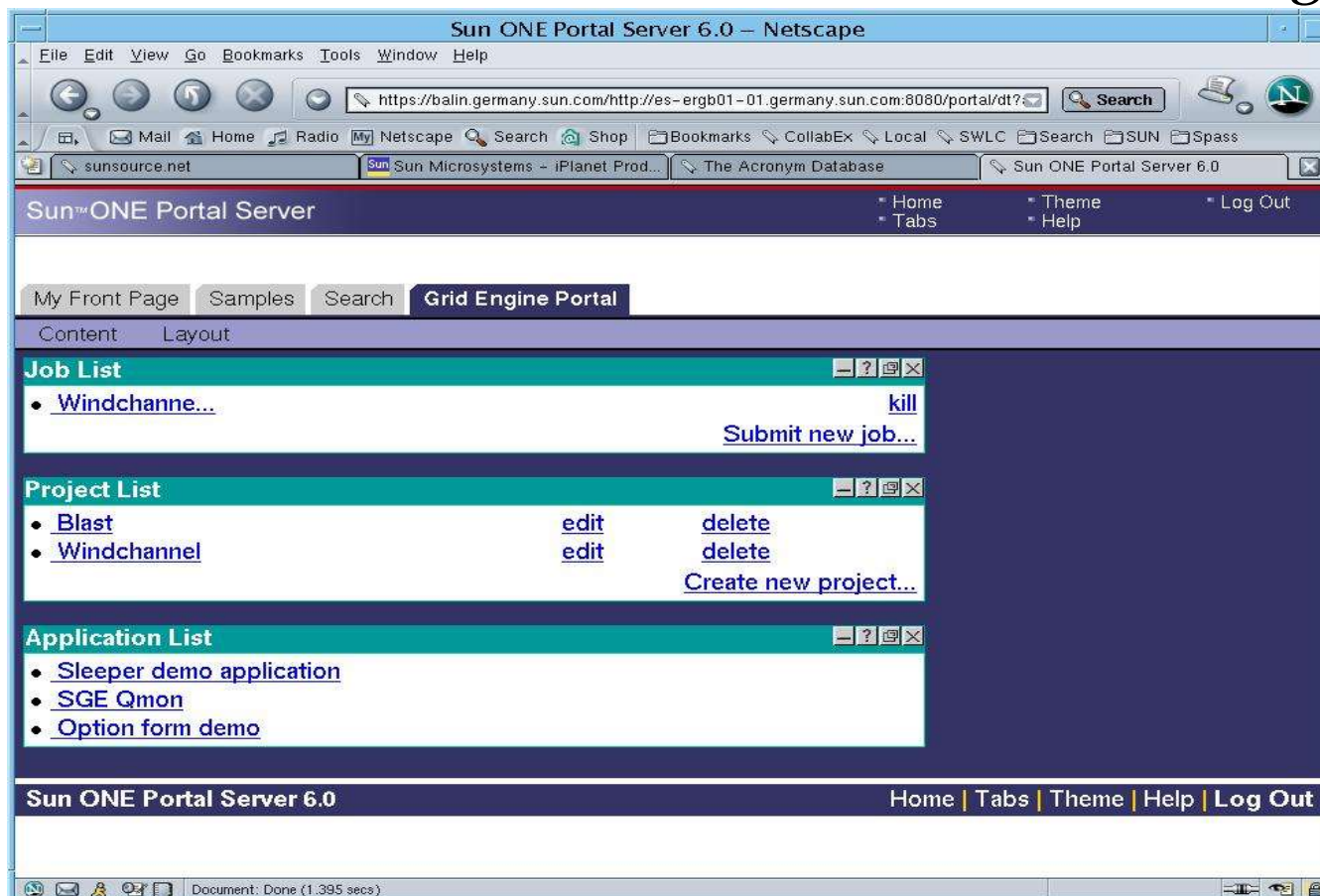


Supports
Solaris, Linux,
and Other
Operating Systems

Grid Interface:

Access to Web-based HPTC Services

Sun ONE Grid Portal: A Sun PS Offering



The screenshot shows a Netscape browser window displaying the Sun ONE Portal Server 6.0 interface. The browser's address bar shows the URL: <https://balin.germany.sun.com/http://es-ergb01-01.germany.sun.com:8080/portal/dt?>. The browser's menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The browser's toolbar includes navigation buttons, a search box, and a search button. The browser's status bar shows the document is done in 1.395 seconds.

The Sun ONE Portal Server 6.0 interface is displayed in a dark blue theme. The top navigation bar includes links for Home, Theme, Log Out, Tabs, and Help. Below the navigation bar, there are tabs for My Front Page, Samples, Search, and Grid Engine Portal. The Grid Engine Portal tab is selected. Below the tabs, there are sections for Job List, Project List, and Application List. Each section has a title bar with a close button and a list of items with associated actions.

Job List

- [Windchanne...](#) [kill](#)

[Submit new job...](#)

Project List

Blast	edit	delete
Windchannel	edit	delete

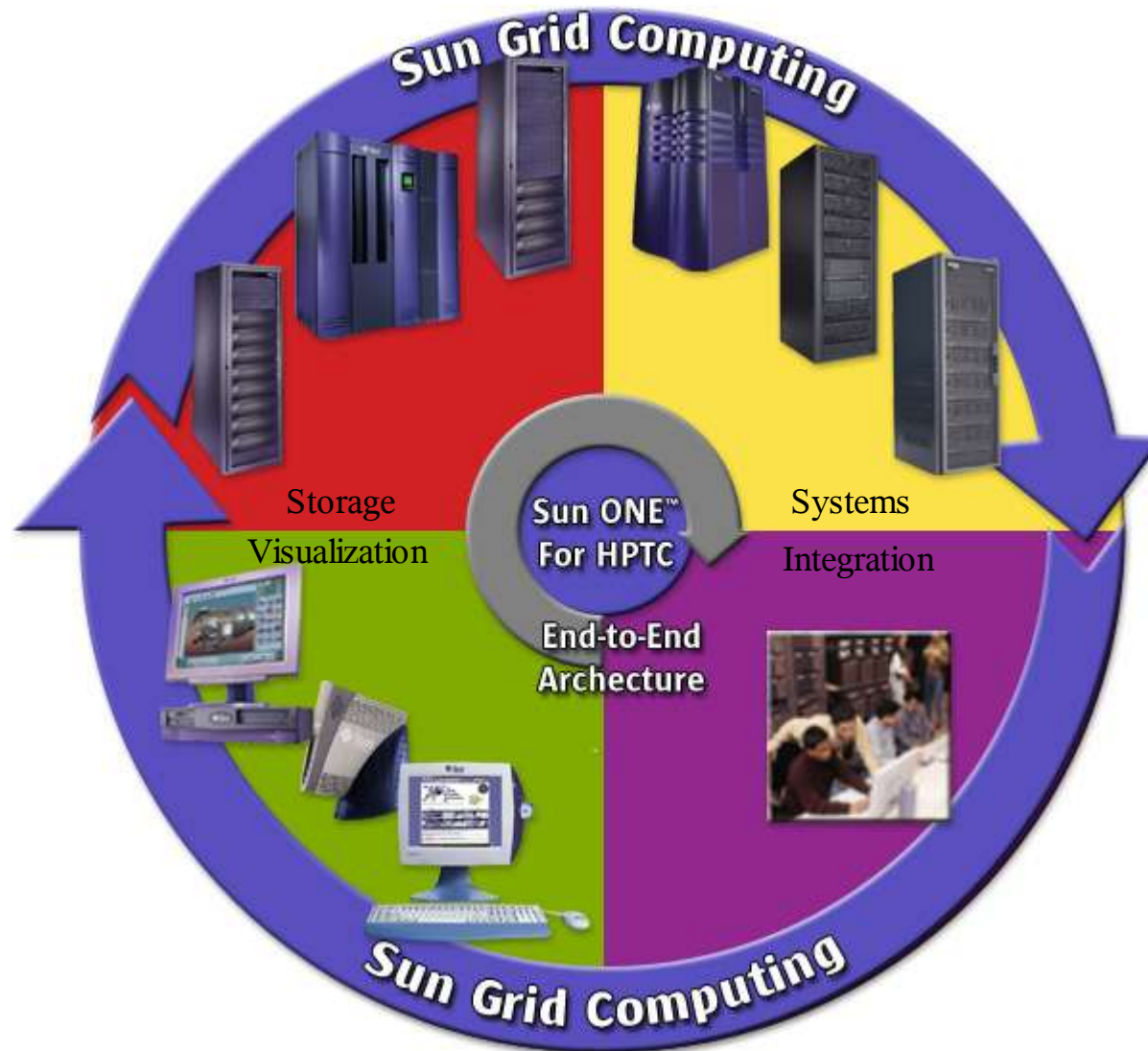
[Create new project...](#)

Application List

- [Sleeper demo application](#)
- [SGE Qmon](#)
- [Option form demo](#)

The bottom of the page features a footer with the text "Sun ONE Portal Server 6.0" and navigation links for Home, Tabs, Theme, Help, and Log Out.

Sun's HPTC Strategy



Asia Pacific Science and Technology Centers

Objectives

- To provide technical and scientific expertise for technical computing business
- To conduct Applied Research in Science and Engineering

Focus Area

Life Science
Computing

Engineering
Computing

Financial
Computing

Mathematical
Science
and
Modelling

GRID Computing

HPTC Environment

Performance Tuning

Status FY04

- Singapore Center is opened in December 2002
- Japan Center will be announced Soon !
- China Center is still in planning stage
- India and Malaysia Facilities are up and running
-

Status FY04

- Singapore Center
 - Collaboration and Projects
 - BioBox (in discussion)
 - A/Prof Tan Tin Wee
 - Financial Engineering (still in discussion)
 - Prof Kah and Prof Lee (NUS)
 - Reliable Computing
 - Prof Liew Kim-Meow
 - Game Theory
 - Prof Robert Gay
 - AIST on APGRID
 - MOU with APBioNet

Support to other industries

- Defense
 - Benchmarking
- Manufacturing
 - Porting and Grid Implementation
- Finance and Banking
 - In progress

ApGrid Branch in Sun's Booth



on the ApGrid Testbed

Ultra Enterprise Cluster



Sun Grid Engine
(AIST, Japan)



622Mbps x 2

Sun Demo Station



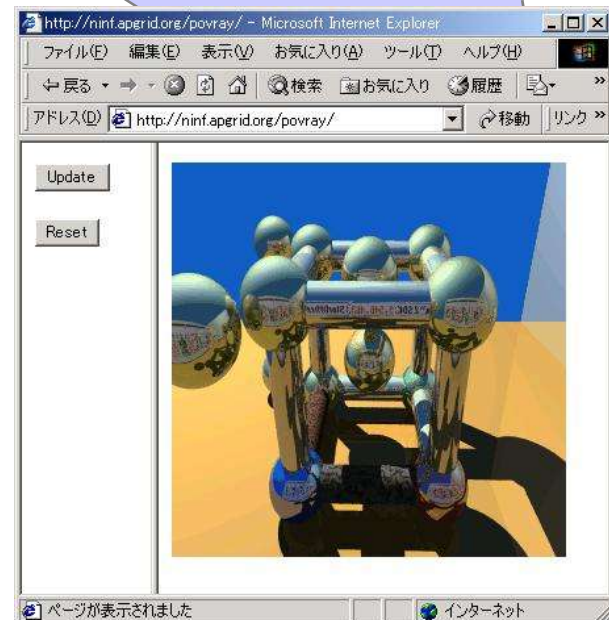
Denver, USA

Job submission using

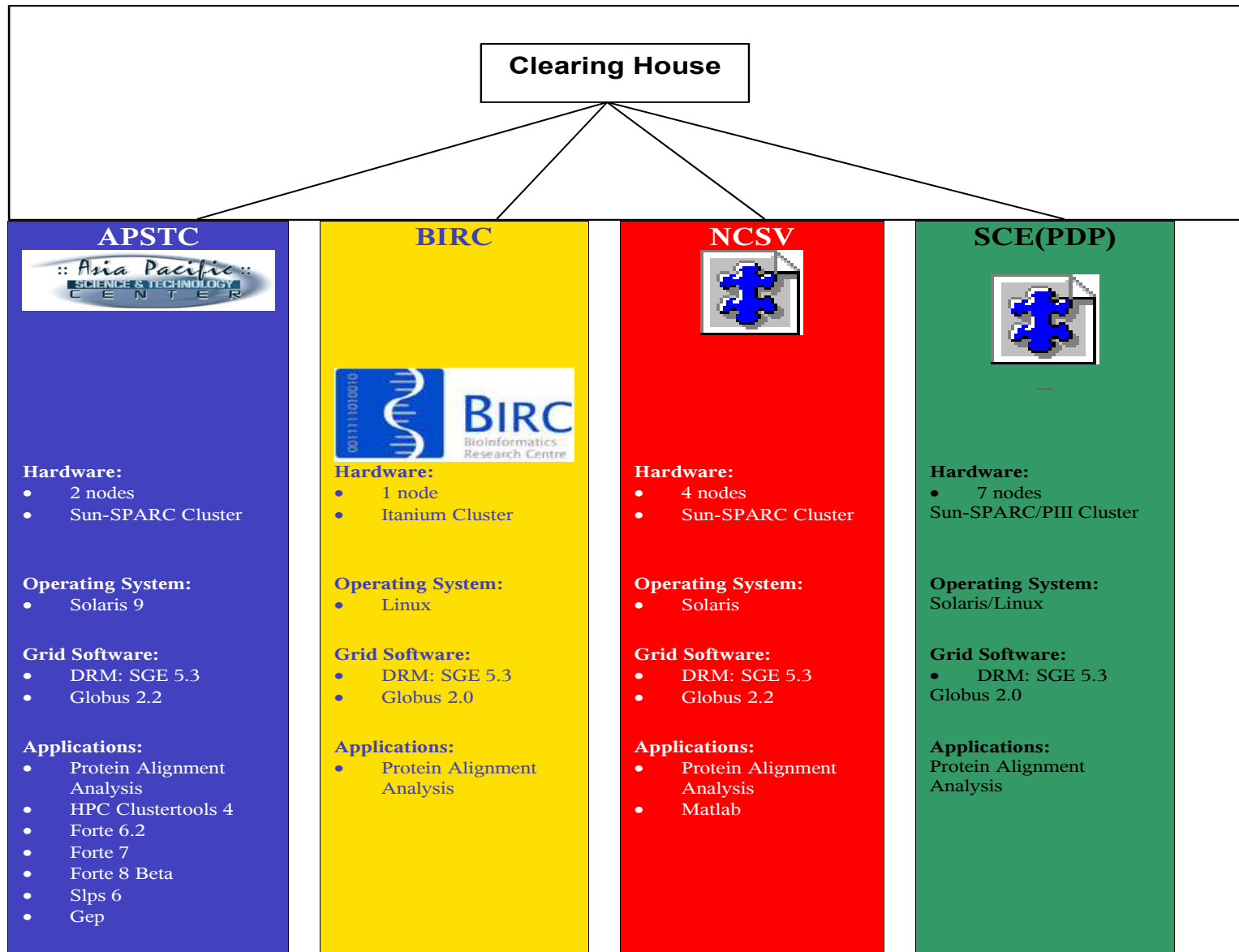


Globus

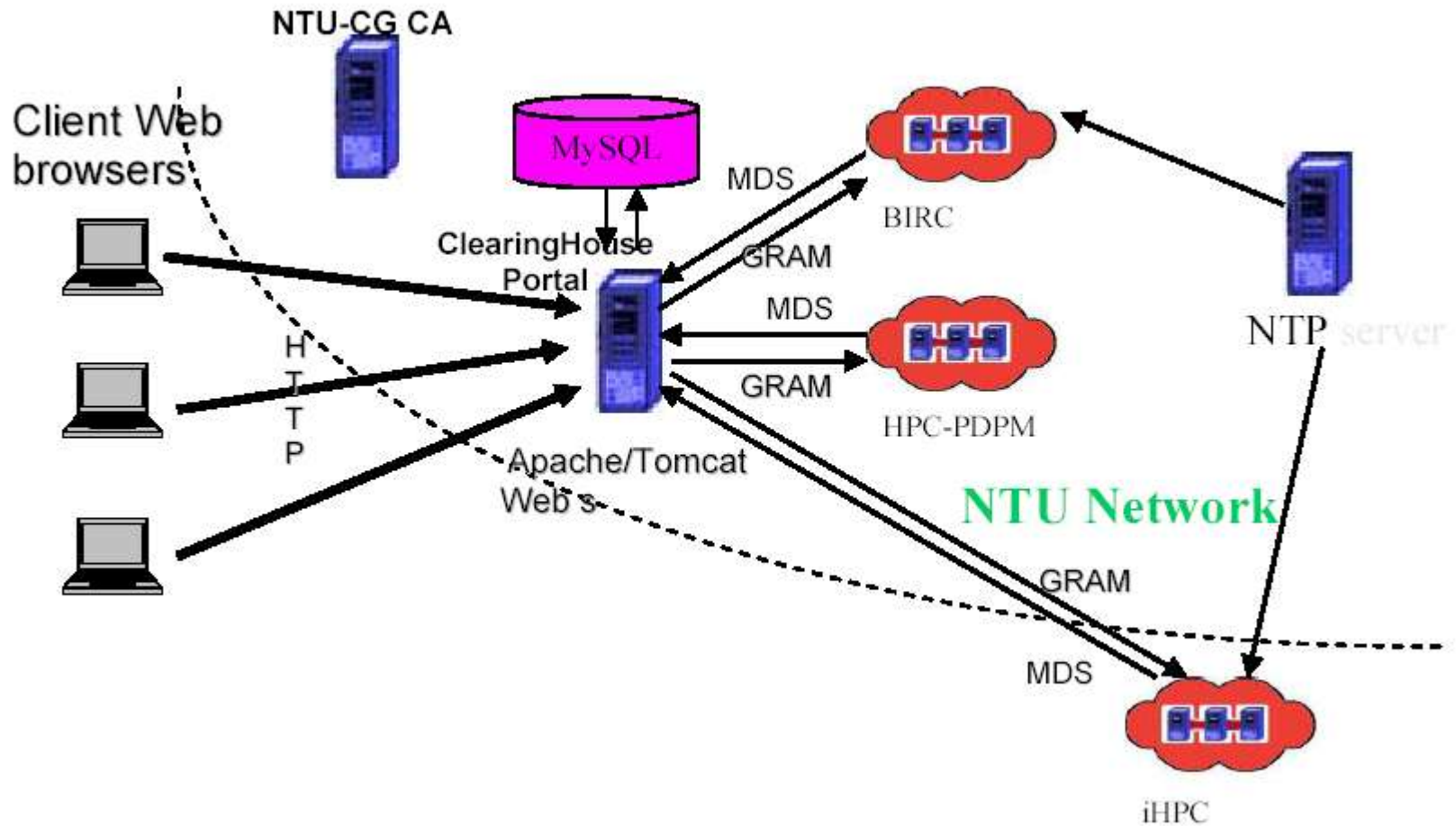
the globus project™
www.globus.org



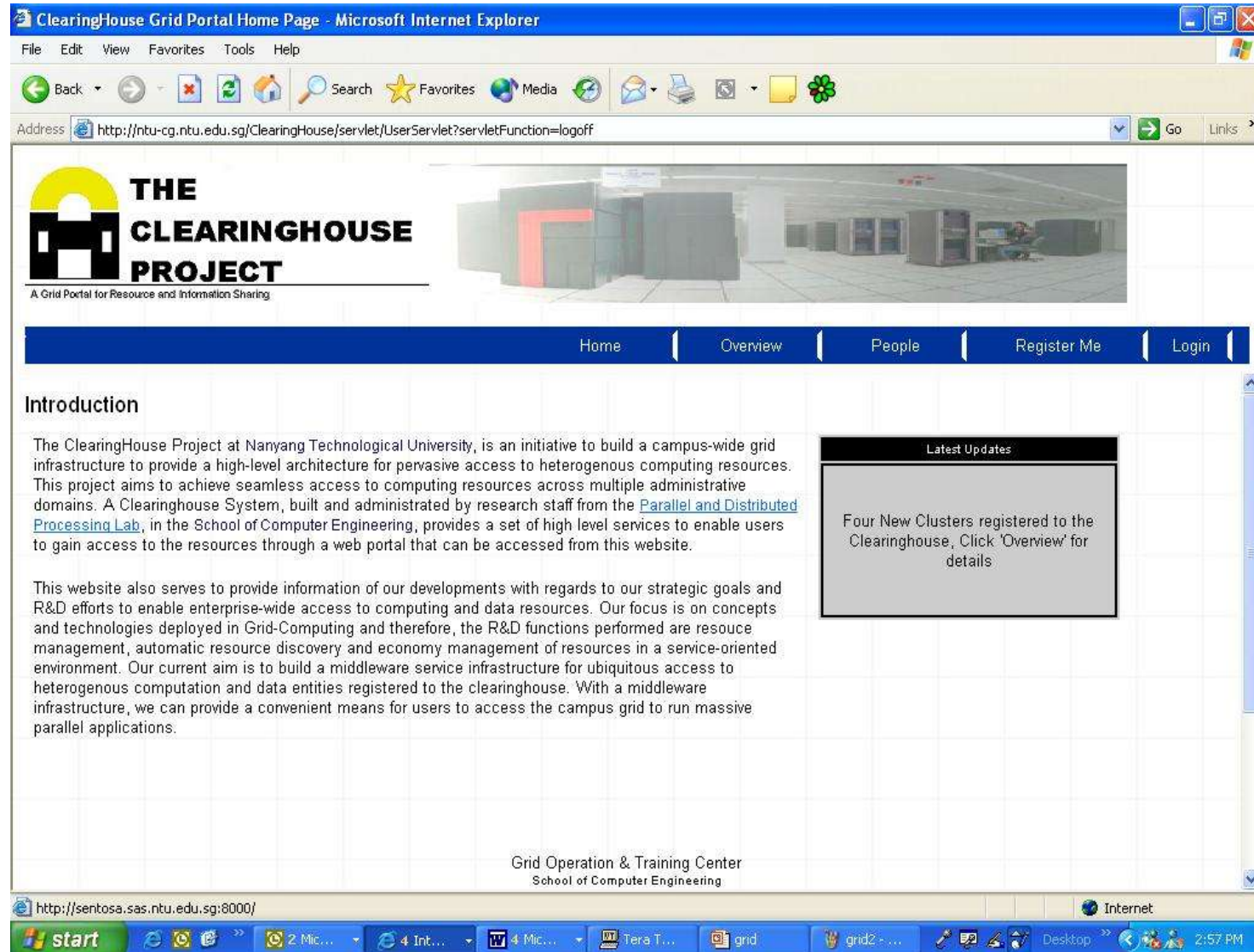
NTU-CampusGrid



Campus Grid Connectivity



www.ntu-cg.ntu.edu.sg



ClearingHouse Grid Portal Home Page - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://ntu-cg.ntu.edu.sg/ClearingHouse/servlet/UserServlet?servletFunction=logout> Go Links >>

THE CLEARINGHOUSE PROJECT

A Grid Portal for Resource and Information Sharing

Home | Overview | People | Register Me | Login

Introduction

The ClearingHouse Project at Nanyang Technological University, is an initiative to build a campus-wide grid infrastructure to provide a high-level architecture for pervasive access to heterogenous computing resources. This project aims to achieve seamless access to computing resources across multiple administrative domains. A Clearinghouse System, built and administrated by research staff from the [Parallel and Distributed Processing Lab](#), in the School of Computer Engineering, provides a set of high level services to enable users to gain access to the resources through a web portal that can be accessed from this website.

This website also serves to provide information of our developments with regards to our strategic goals and R&D efforts to enable enterprise-wide access to computing and data resources. Our focus is on concepts and technologies deployed in Grid-Computing and therefore, the R&D functions performed are resource management, automatic resource discovery and economy management of resources in a service-oriented environment. Our current aim is to build a middleware service infrastructure for ubiquitous access to heterogenous computation and data entities registered to the clearinghouse. With a middleware infrastructure, we can provide a convenient means for users to access the campus grid to run massive parallel applications.

Latest Updates

Four New Clusters registered to the Clearinghouse, Click 'Overview' for details

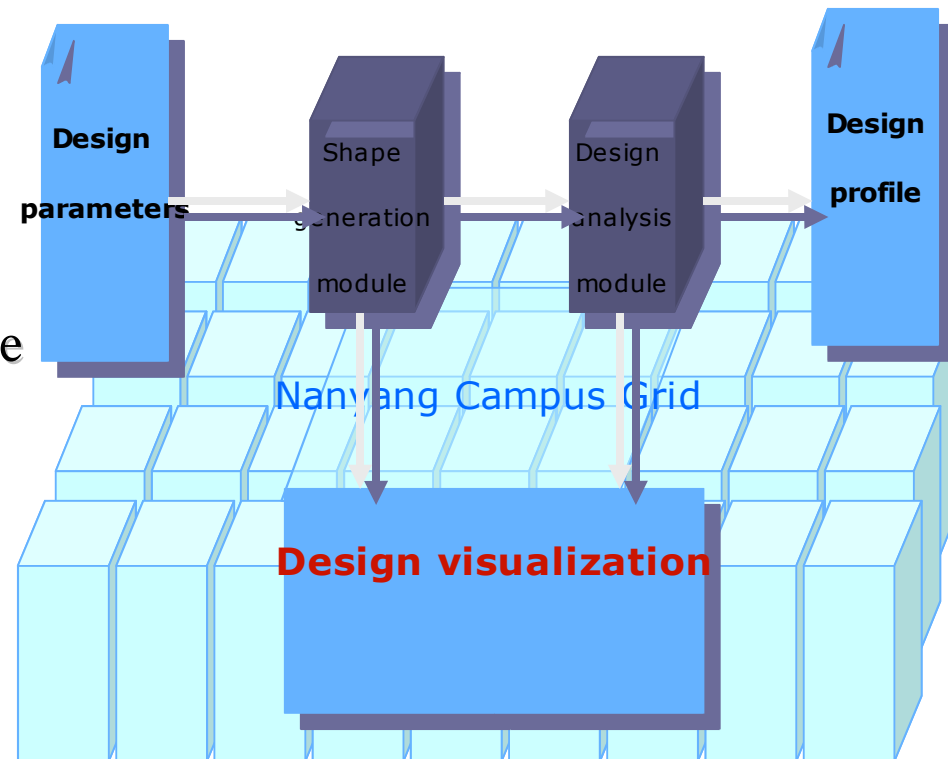
Grid Operation & Training Center
School of Computer Engineering

Internet

start 2 Mic... 4 Int... 4 Mic... Tera T... grid grid2 - ... Desktop 2:57 PM

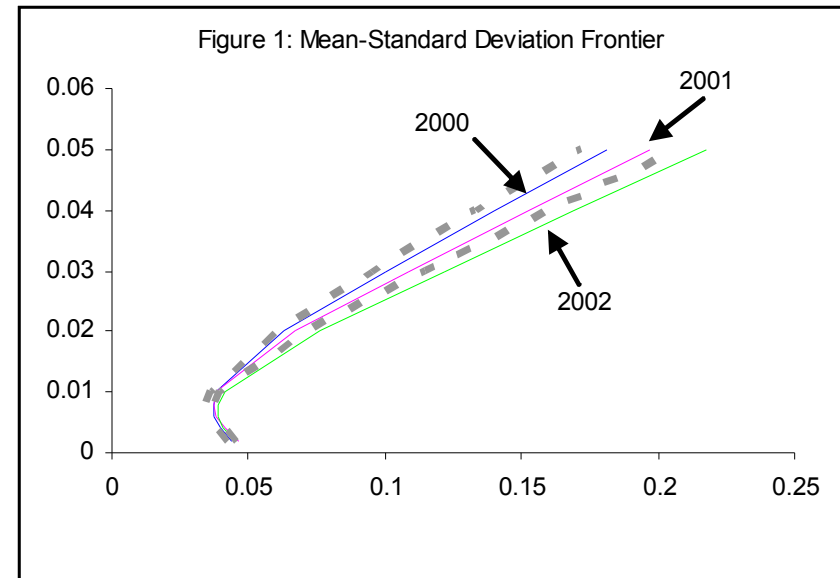
Design Grid Problem Solving Environment

This project vision provides an Internet portal giving remote access to general analysis and design tools. Our development road map for this takes a route initially for Computational Fluid Dynamic, Finite Element and Multi-disciplinary Analysis and Design Grid Optimisation for a diverse of science and engineering applications.



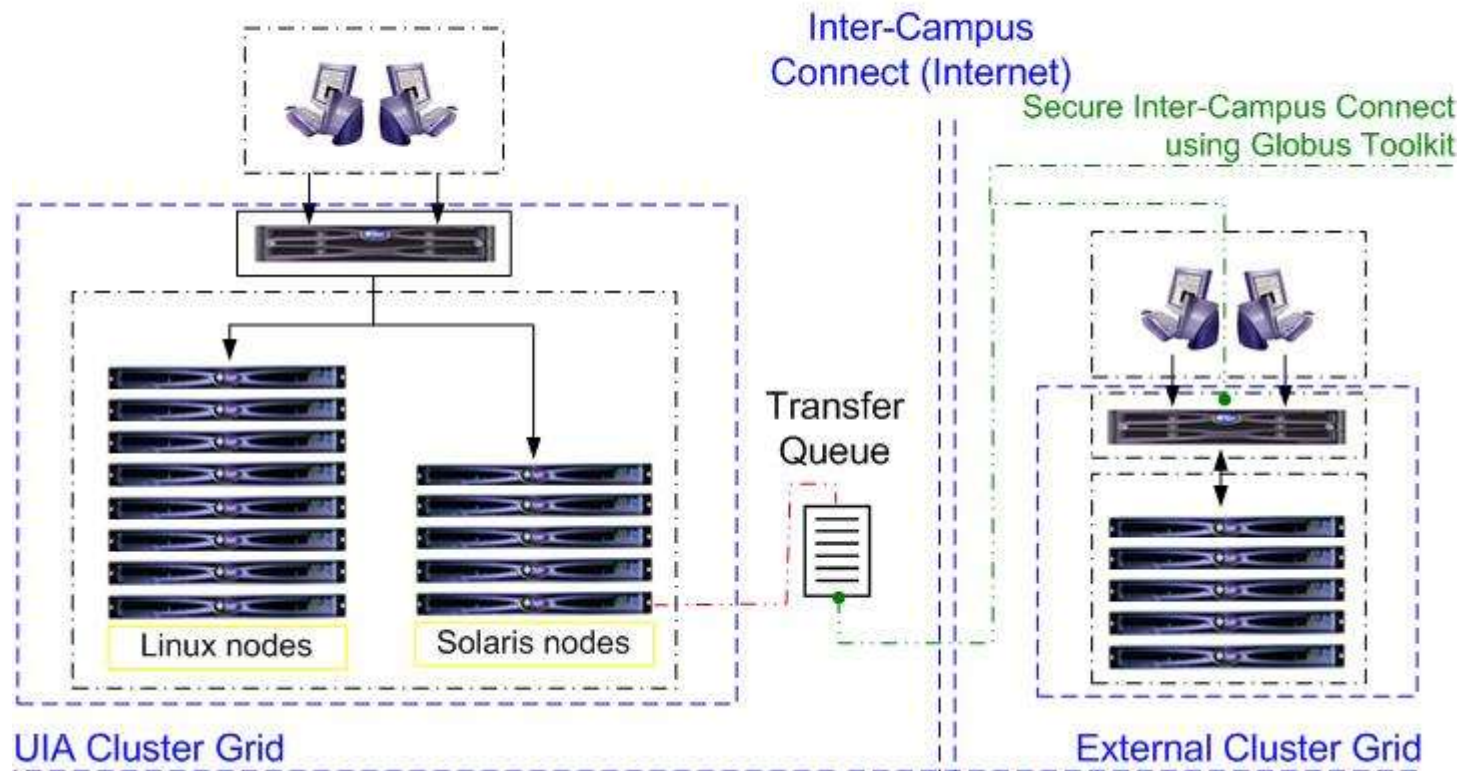
Portfolio Rebalancing in a Grid Computing Framework

- We present an approach to compute the efficient frontier for portfolio optimization based on evolutionary programming (EP) technique. Our approach relies on multiple EP runs within a search to create the frontier.



USM/UKM Grid

Heterogeneous Inter-Cluster Proposal Setup



Collaborative R/D

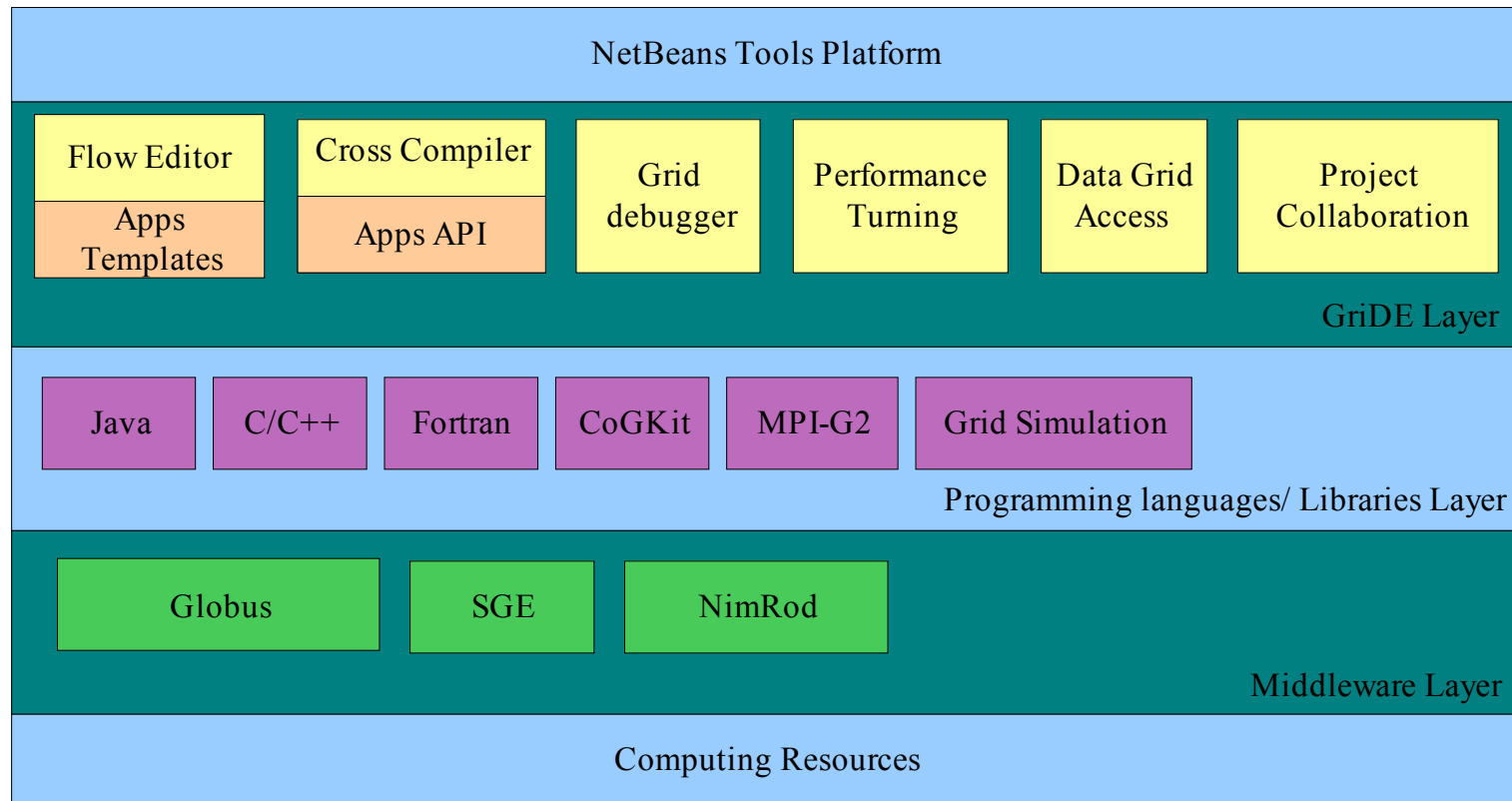
- Grid Computing
 - Development of Tools, scheduling algorithms, middleware
 - Grid IDE, Superscheduler.....
 - and large scale implementation
 - NTU-Campus Grid
 - Singapore National Grid
 - Asia Pacific Grid (APGrid)

GriDE Overview

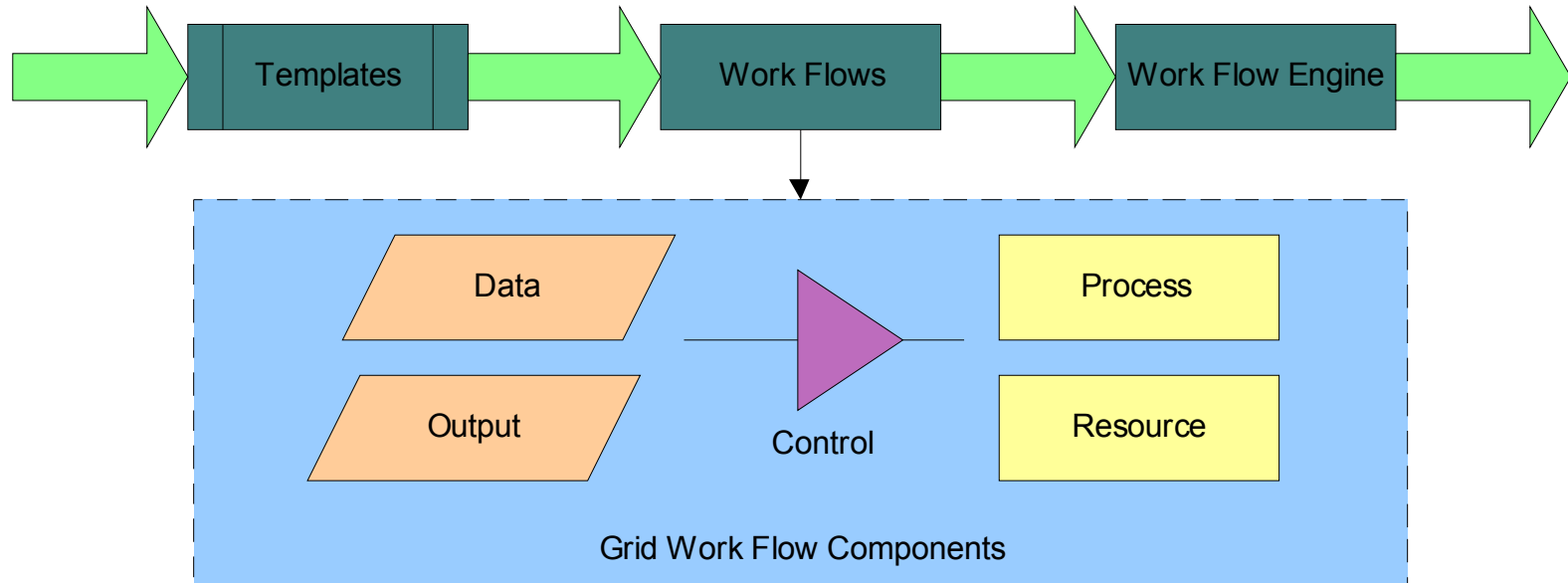
GriDE is an integrated development environment that make it straightforward for scientists and engineers to construct grid applications. It provides friendly tools to access grid resources and makes the development approach easily and fast.

- Portability
- Scalability
- Convenience
- Modular
- Security
- Transparency

GriDE Architecture



GUI based Flow Editor



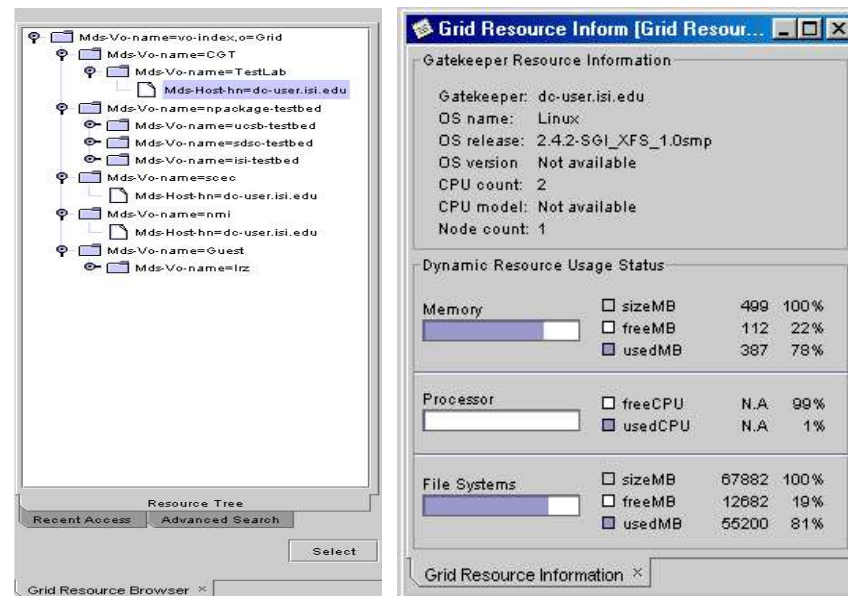
Based on the predefined templates and grid components, the developers can easily define the work flow of their grid applications. It will automatically compiled by the work flow engine which generates the script or source codes to execute or deploy the application to the grid.

Grid Debugger (1)

Grid Debugger includes the tools to browse the grid resources, execute applications and debug on a grid simulation environment.

Resource Browser

- easy to explore Grid resources
- Monitor the resource usage

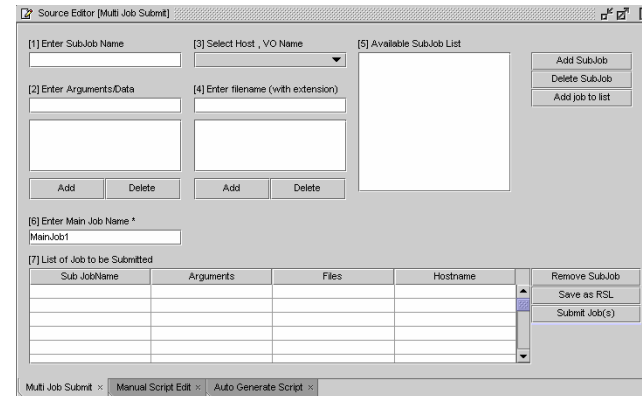


Grid Debugger (2)

Hierarchical Job Submission

– Convenient submit anywhere

you can



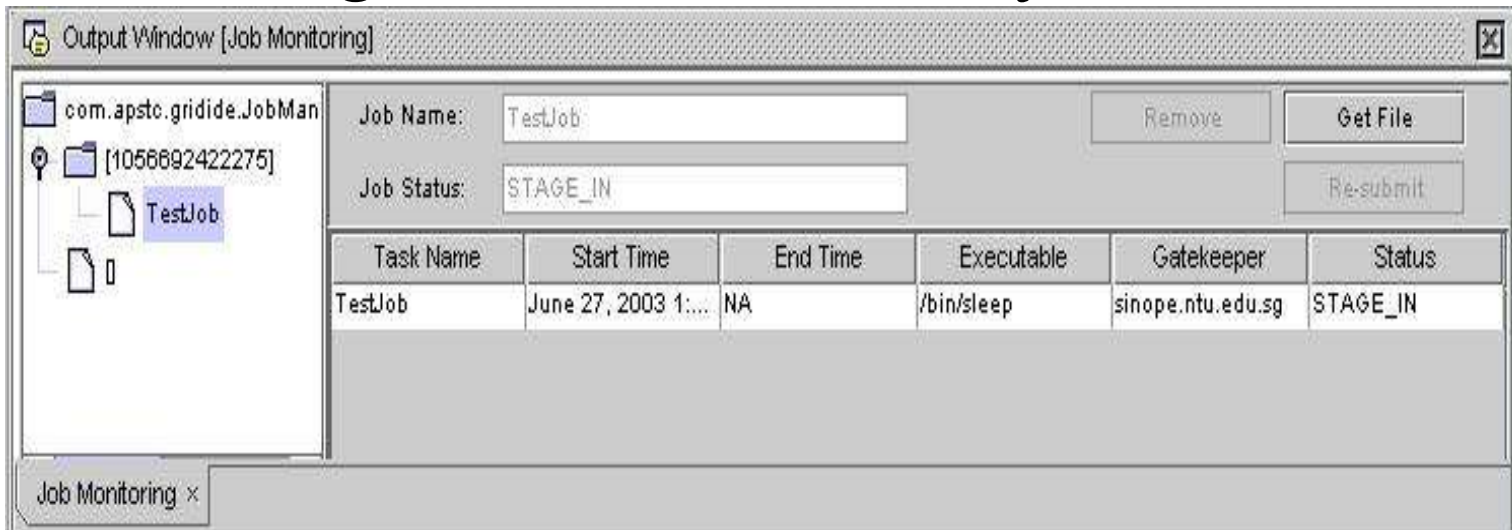
- Quick Job Submit

- Multiple Job Submit

Grid Debugger (3)

Job Monitoring

- Retrieve detail job execution information
- Tracking the execution history



Output Window [Job Monitoring]

com.apstc.gridide.JobMan

[1056692422275]

TestJob

Job Name: TestJob

Job Status: STAGE_IN

Remove Get File

Re-submit

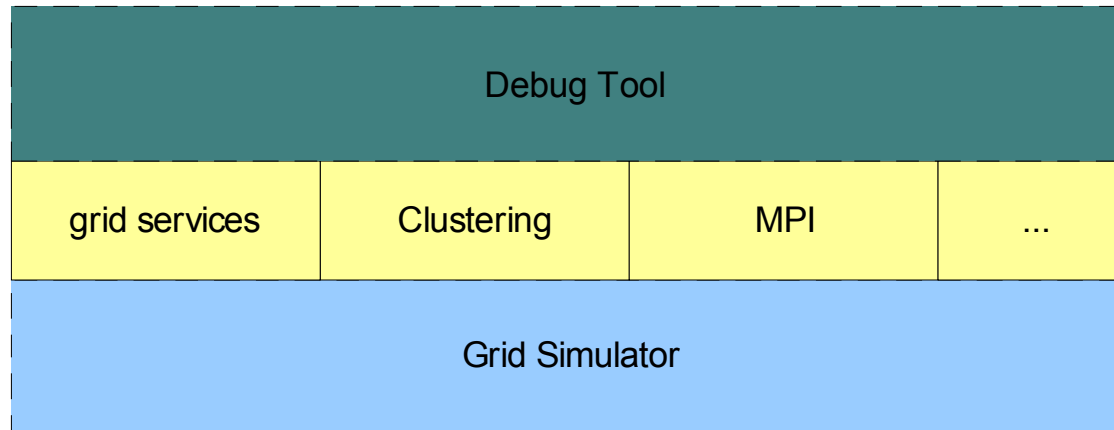
Task Name	Start Time	End Time	Executable	Gatekeeper	Status
TestJob	June 27, 2003 1:...	NA	/bin/sleep	sinope.ntu.edu.sg	STAGE_IN

Job Monitoring x

Grid Debugger (4)

Debugger

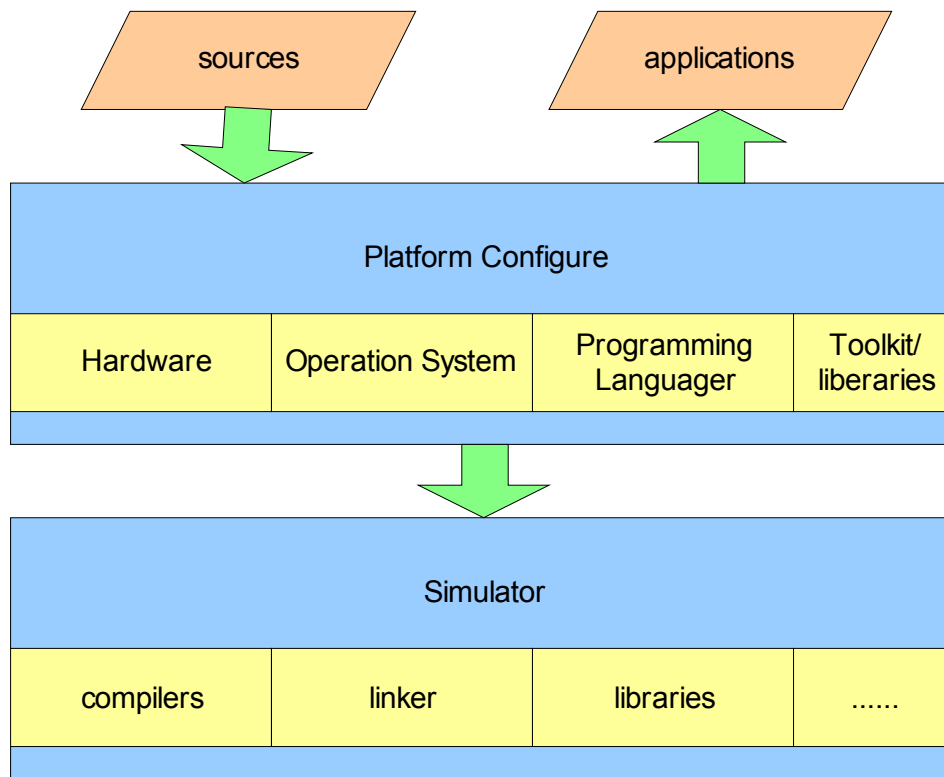
- Execute in the grid simulation environment
- Debug for parallel applications, and grid services



Performance Tuning

- Monitor grid resource usage
- Monitor execution performance
- Dynamically select resources
- Migrate applications between different resources

Cross Compiler



- Compile for multiple programming languages
- Compile for different operation systems
- Compile for different hardware

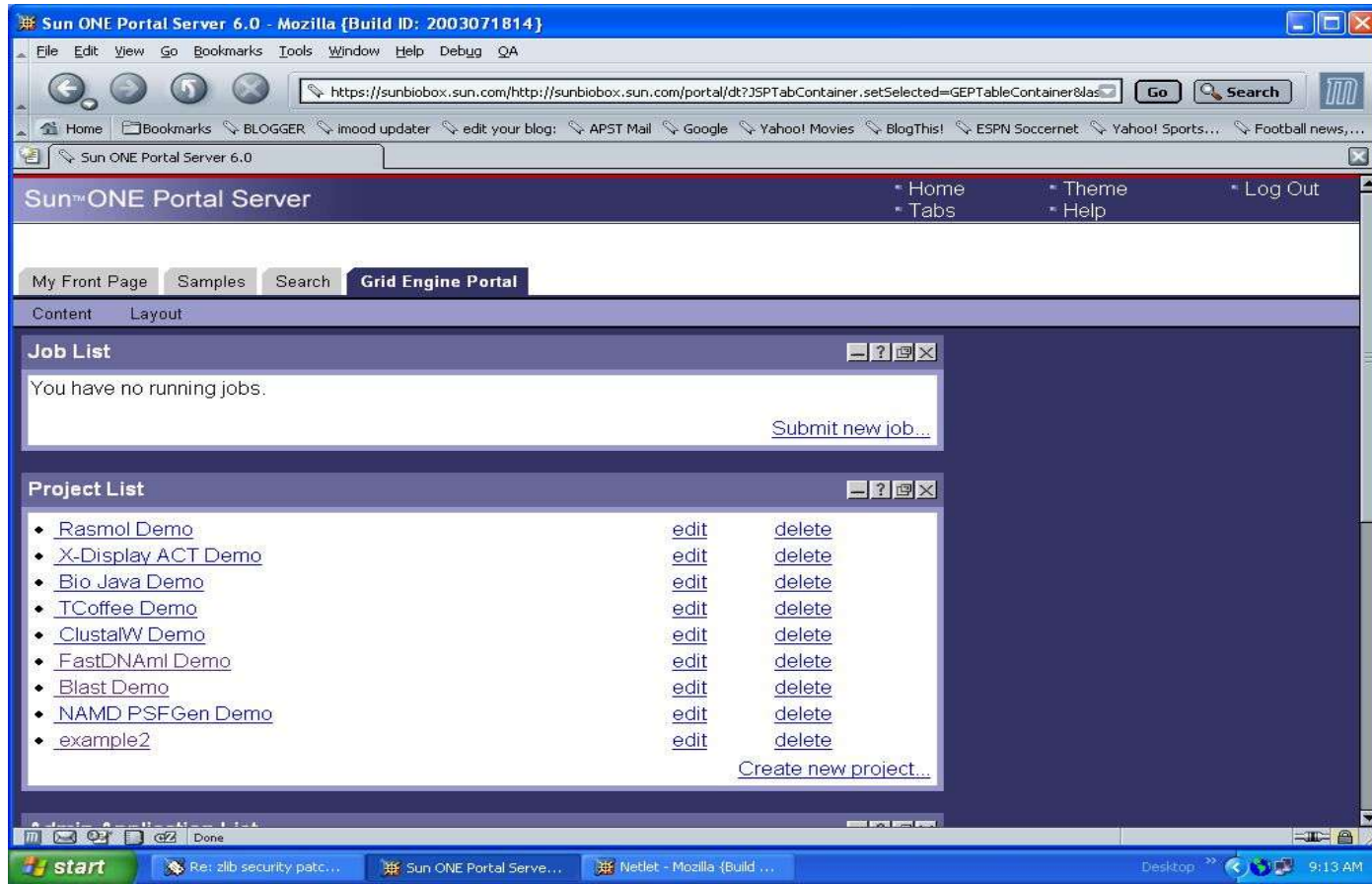
Collaborative R/D

- Life Science
 - Workflow Engineering
 - Intergration of Portal, Life Science Applications and Grid.
 - Life Science Package (BioBox)
 - Algorithms
 - Work with researchers on new algorithms and map them to Sun platform. Optimization and tuning.

What is the BioBox?

- Easy-to-deploy installation package consisting of Sun OS and most popular Biox applications.
- Users who aren't familiar or want to avoid compilation/installation of OS/Biox applications.

Submitting BLAST job using GEP



Application Categories

- Homology & Similarity Search (Blast)
- Sequence Analysis (Hmmer)
- Structural Prediction (Phylip)
- Molecular Imaging/Modeling(NAMD)
- Others (Biojava)

Deployment Architecture of Bio-ClusterGrid

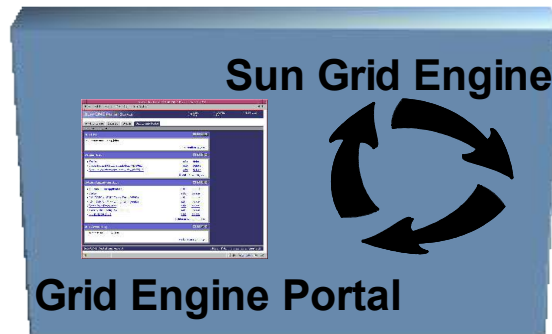
Bioinformatics Applications

Homology and Similarity Search: Biodas, BLAST, FASTA, GlimmerM, Wise
 Sequence Analysis: ACT, ClusterW, EMBOSS, HMMER, Image, T-Coffee
 Structural Prediction: DOWSER, FastDNAmI, LOOPP, MapMaker/QTL, PAML, PHYLIP
 Molecular Imaging/Modeling: Artemis, Cn3D, GROMACS, NAMD, NMRView, RasMol, ReadSeq, TribeMCL, VMD
 Others: Biojava, Bioperl, Biopython



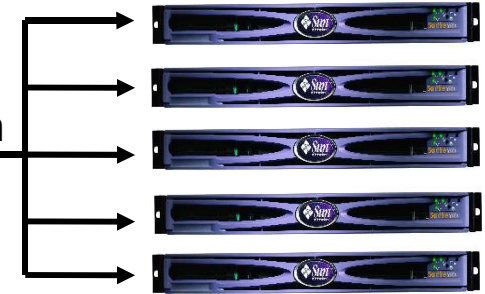
← Results

Jobs →



Cluster of Execution Hosts

Dispatch



Functional Description

Access Tier - users access via browser (GEP)

Hardware

Sun Ray Thin Client + Sparc Solaris Sunray Server

Software

Sunray Server 2.0

Or other desktop operating systems

Functional Description

Resource Management/Portal Tier
 GEP provides entry point for job submission
 SGE schedules jobs to execution hosts
 SGE monitors job status/completion of jobs
 GEP presents job status/results to users
 SCE/GEP server acts as file server

Hardware

1 x SFV240 Sparc Server (2 cpu, 2GB)

Software

Solaris 9, Sun Grid Engine, Grid Engine Portal
 Customer/ISV applications
 HPC Cluster Tools, SunOne Studio 8 Compiler

Functional Description

Execution Tier (execution hosts)
 Executes jobs sent to it by Grid Master Hosts
 Returns job status/results to Grid Master Hosts

Hardware

SFV210 Sparc Server (2 cpu, 2GB) - multiple nodes

Software

Solaris 9, Sun Grid Engine, Grid Engine Portal
 Customer/ISV applications
 HPC Cluster Tools, SunOne Studio 8 Compiler

Collaborative R/D

- Physical Science and Engineering
 - Workflow Engineering
 - Intergration of Portal, Applications , Grid and collaborative environment
 - Algorithms
 - Work with researchers on new algorithms and map them to Sun platform. Optimization and tuning.

Research in Reliable computing

- “Rate of progress toward the *correct answer.*”
- Implications:
 - Measuring floating-point “performance” is problematic.
 - Convergence everywhere to the wrong answer is *not* helpful!

F/P examples /1

Mathematically:

$$\begin{aligned}x &= (10^{20}) \times (0.1 - 3 * (0.1/3)) \\ &= 0\end{aligned}$$

$$y = (10^{20} + 1) - 10^{20}$$

F/P examples /2

$$X = (10^{**}20) * (.1 - 3. * (.1 / 3.))$$

$$= -.7450580746E+12$$

? 0

$$Y = (10^{**}20 + 1) - 10^{**}20$$

$$= 0.000000000000E+00$$

? 1

Example: Big \times Small

$$x = \text{Big} \times \text{Small}$$

$$\text{Big} = 10^{20}$$

$$\text{Small} = 0.1 - 3 \times (0.1/3)$$

$$\text{Right answer: } x = 0$$

Ex: Big1 – Big2

$$y = \text{Big1} - \text{Big2}$$

$$\text{Big1} = 10^{20} + 1.$$

$$\text{Big2} = 10^{20}$$

Right answer: $y = 1$

Using F/P

! Copyright 03/25/2003 Sun Microsystems, Inc.

```
REAL(4)      BIG,  X,  Y
```

```
BIG = 1.0E+20
```

```
X   = BIG * ( .1 - 3. * (.1/3.))
```

```
Y   = (BIG + 1.) - BIG
```

```
PRINT ' (" X = ", E20.10, ", Y = ", E20.10) ',  
X, Y
```

```
PRINT '(1X)'
```

END

Using F/P

! Copyright 03/25/2003 Sun Microsystems, Inc.

```
REAL(4)      BIG,  X,  Y
```

```
BIG = 1.0E+20
```

```
X   = BIG * ( .1 - 3. * (.1/3.))
```

```
Y   = (BIG + 1.) - BIG
```

```
PRINT '( " X = ", E20.10, ", Y = ", E20.10 )',  
X, Y
```

```
PRINT '(1X)'
```

END

Interval Definition

- Represented as $[a,b]$ or $[2,3]$
 - A continuous set of numbers bounded by its endpoints $a \leq b$ (or $2 \leq 3$)

Interval Definition

- Represented as $[a,b]$ or $[2,3]$
 - A continuous set of numbers bounded by its endpoints $a \leq b$ (or $2 \leq 3$)
 - Formally:

Containment set (cset)

$$[a, b] = \bigcup_{a \leq x \leq b} x$$

$$= \{x \mid a \leq x \leq b\} \text{ where}$$

$$a \text{ and } b \in \mathbb{R} = (-\infty, +\infty).$$

Basic Arithmetic Operations

$$[a, b] + [c, d] = [a + c, b + d]$$

$$[a, b] - [c, d] = [a - d, b - c]$$

$$[a, b] \times [c, d] = \begin{bmatrix} \min(a \times c, a \times d, b \times c, b \times d) \\ \max(a \times c, a \times d, b \times c, b \times d) \end{bmatrix}$$

$$[a, b] \div [c, d] = \begin{bmatrix} \min(a \div c, a \div d, b \div c, b \div d) \\ \max(a \div c, a \div d, b \div c, b \div d) \end{bmatrix}$$

given $d < 0$, or $0 < a$.

Using F/P + intervals

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```
REAL(4)      BIG, X, Y
```

```
INTERVAL(4) BIGI, XI, YI
```

```
BIG = 1.0E+20
```

```
X = BIG * (.1 - 3. * (.1/3.))
```

```
Y = (BIG + 1.) - BIG
```

```
PRINT '( " X = ", E20.10, ", Y = ", E20.10)',  
X, Y
```

```
PRINT '(1X)'
```

```
BIGI = 1.0E+20
```

```
XI = BIGI * (.1 - 3 * (.1/3))
```

Results

F/P:

$$\mathbf{X} = -0.7450580746\mathbf{E}+12$$

$$\mathbf{Y} = 0.0000000000\mathbf{E}+00$$

Intervals:

$$\mathbf{XI} = [-0.3\mathbf{E}-14, 0.3\mathbf{E}-14]$$

$$\mathbf{YI} = [-0.9\mathbf{E}+13, 0.9\mathbf{E}+13]$$

Interval Benefits

- Good representation of physical reality
 - Visible accuracy and uncertainty information
 - $x \in [2.3, 3.5] \implies 2.3 \leq x \leq 3.5$
 - Measurement error/uncertainty
 - Rigorous error/sensitivity analysis
 - Machine interval: the set of **all** points therein
 - Intervals are compact sets (or continua)
- Elegant and fast system hardware and software
 - No exceptional events
 - Algebraically closed real and complex number systems
 - No singularities: division by zero
 - No indeterminate forms: $0/0$ $\infty - \infty$ and $0 \times \infty$

Reliable Computing

- Limited precision in current computing paradigm
 - Imprecise computation
 - Unreliable result
- New Computing Paradigm
 - Interval Arithmetics
- Interval Arithmetics
 - Represent FP in bounded by Interval
- New Algorithm

Other Research Collaboration

- GIS
 - Digital Biologist
- SBS/NTU
 - Bio/Med Grid
- USM/UKM
 - Bio Grid
- BioTec (Thailand)
 - Bio Cluster and BioX Applications
- ASIT (Philippines)
 - Biobox initiative (training)
- University of Hokkiado
- KRIBB (Korea)
- Univ of Queensland (Aus)

Paper Published

- *A Sort-First Parallel Rendering Algorithm for Distributed Rendering Environments*, Huabing Zhu, Kai Yun Chan, Lizhe Wang, Wen Tong Cai & Simon See, Cyberworlds 2003, Singapore, 3-5 December 2003.
- *A Resource Co-reservation Heuristic for Parallel Tasks in Computational Grids*, Lizhe Wang, Wentong Cai, Simon See & Wei Jie, Parallel Computing 2003 (ParCo2003), 2-5 September 2003.
- *Packet Triplet: An enhanced packet pair probing for path capacity estimation*, Jie Song, Proceedings of Network Research Workshop, pp. 93-97, Busan, Republic of Korea, 27 August 2003.
- *Resource Co-allocation for Parallel Tasks in Computational Grids*, Lizhe Wang, Wentong Cai, Bu-Sung Lee, Simon See & Wei Jie, CLADE2003 IEEE HPDC-12 Workshop, 21 June 2003.

Paper Published

- See, S., A Grid-based Technical Computing Portal for MCAE Applications, HPC Asia 2002, Dec 16-19, Bangalore, India
- See, S., Grid Computing with Jini, Jxta and Sun Grid Engine, PDCAT, 2002, Kanazawa.
- See, S., Computer, Internet and Mathematics, Proceeding of second East Asia Regional Conference on Mathematics Education and Ninth Southeast Asian Conference on Mathematics Education, 27-31 May, Singapore
- Pok, V.S., See, S., Thng, I., Use of Rate Control and Historical Data to Improve Performance of Servers, European Simulation Multiconference 2002, 3-5. June 2002, FH-Darmstadt, Germany.
- See, S., Scheduling Algorithm for Distributed Simulation Systems Management, European Simulation Multiconference 2002, 3-5. June 2002, FH-Darmstadt, Germany.

Paper Published (cont)

- See, S., A Distributed Simulation Management Engine For Ordinary Differential Equations, 2002 International Symposium on Parallel Architectures, Algorithms and Networks, I-SPAN2002, Makati City, Metro Manila, Philippines, 22-24 May 2002
- See, S., Interval Arithmetics for Multidisciplinary Design Optimization, MECHANICS & MATERIALS IN DESIGN (M2D-4), 4th International Conference, Nagoya International Center, Nagoya, Japan, June 5 - 8, 2002
- 5 papers are being reviewed for publication

Collaboration

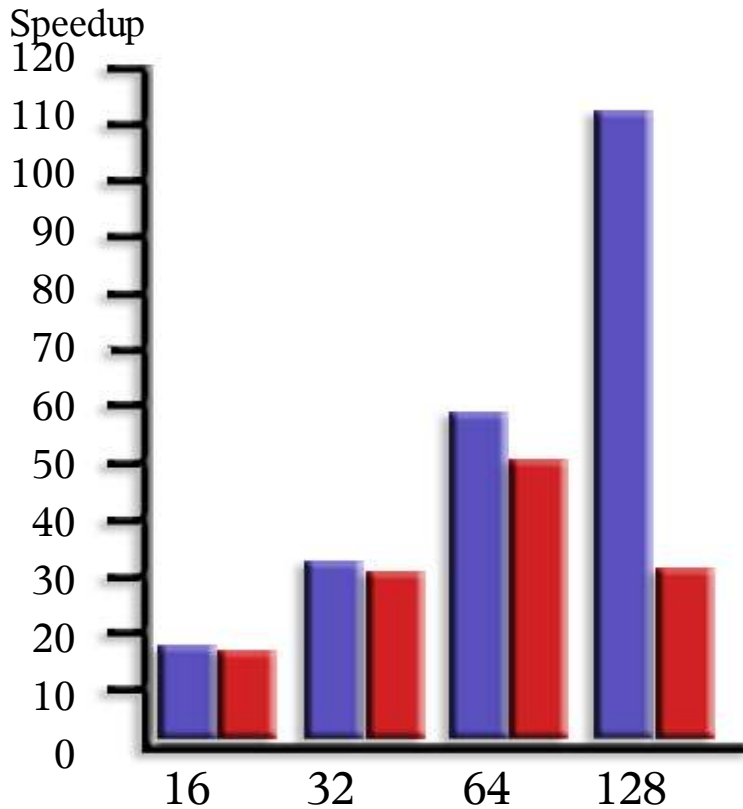
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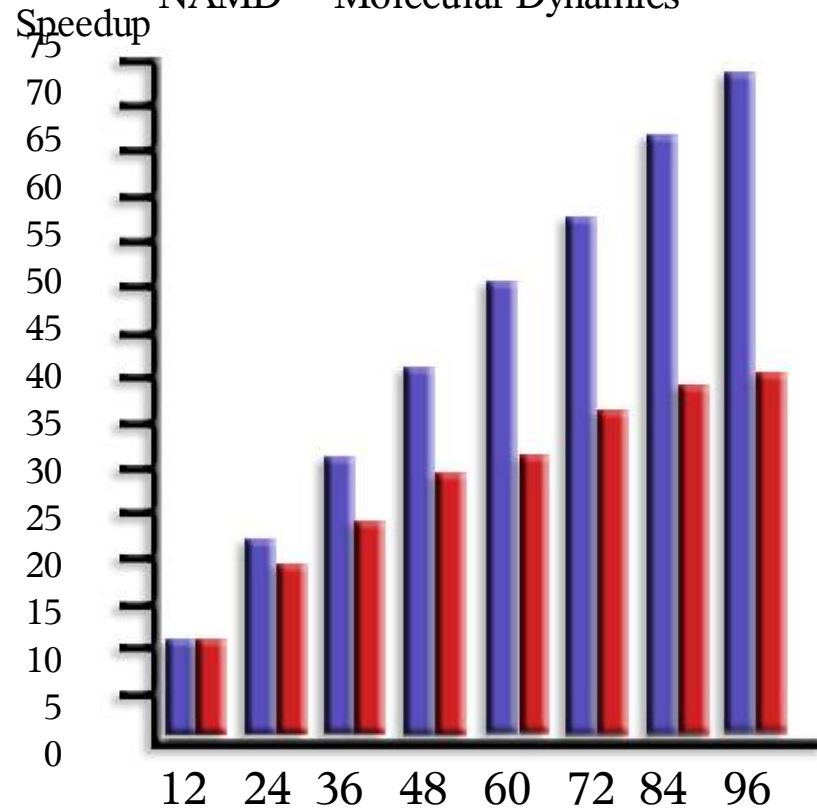
The Interconnect Effect

Sun Fire Link Scalability versus Gbit Ethernet

POP – 8 node Ocean Models



NAMD – Molecular Dynamics



Processors Sun Fire Link (on the left).

Processors

Gbit Ethernet (on the right)