TeraGrid

Charlie Catlett, Director

Pete Beckman, Chief Architect

University of Chicago & Argonne National Laboratory

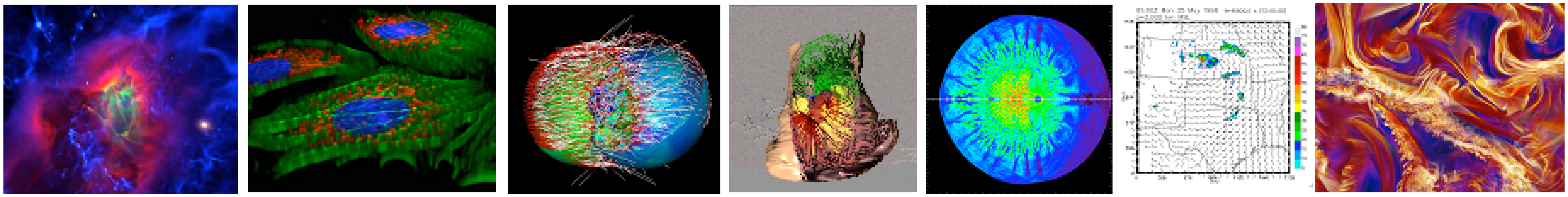
June 2003

GGF-11

Honolulu, Hawaii

The TeraGrid

Distributed resources & expertise can be leveraged to accelerate scientific discovery



Action:

Interconnect large-scale shared scientific databases, computing systems, instruments, and facilities to improve scientific productivity by *removing barriers to collaboration and use of distributed resources*

Funding: US National Science Foundation, industry partners, states
Partners: UC/ANL, Caltech, NCSA, PSC, SDSC, TACC, ORNL, Purdue, Indiana

What we are doing

- Creating a Grid infrastructure that focuses first and foremost on ease of use for users.
  - Common TeraGrid Services & Software (CTSS)
- Creating a software and services infrastructure that is robust and persistent.
  - Inca Verification and Validation System
- Doing this in a way that is easily reproducible and/or extensible
- Not in today's talk… Science Gateways
  - TeraGrid as a wholesale service provider behind discipline-oriented portals, for instance.

Timeline and Program Overview

- Distributed TeraScale Facility (DTF; $50M, 3 yr)
  - IA-64 homogeneous systems at CIT, ANL, NCSA, SDSC
  - Use Grid technologies to embed Grid resources in existing large-scale centers
  - Offer NSF PACI user community a migration path from client-server supercomputing to Grid computing.
- Extensible TeraScale Facility (ETF; $35M, 1 yr)
  - Add Power4 (SDSC), Alpha (PSC) systems
  - Create extensible backbone network (hubs in LA, Chicago)
- TeraGrid Extension Program (TEP; $10M, 1 yr)
  - Add ORNL, TACC, Indiana, Purdue
  - Add network hub in Atlanta
- TeraGrid Operation, Mgmt & Evolution ($150M, 5 yrs)
  - Target date for Production: October 1, 2004 (now in pre-production)
  - TeraGrid OM&E Program currently under review

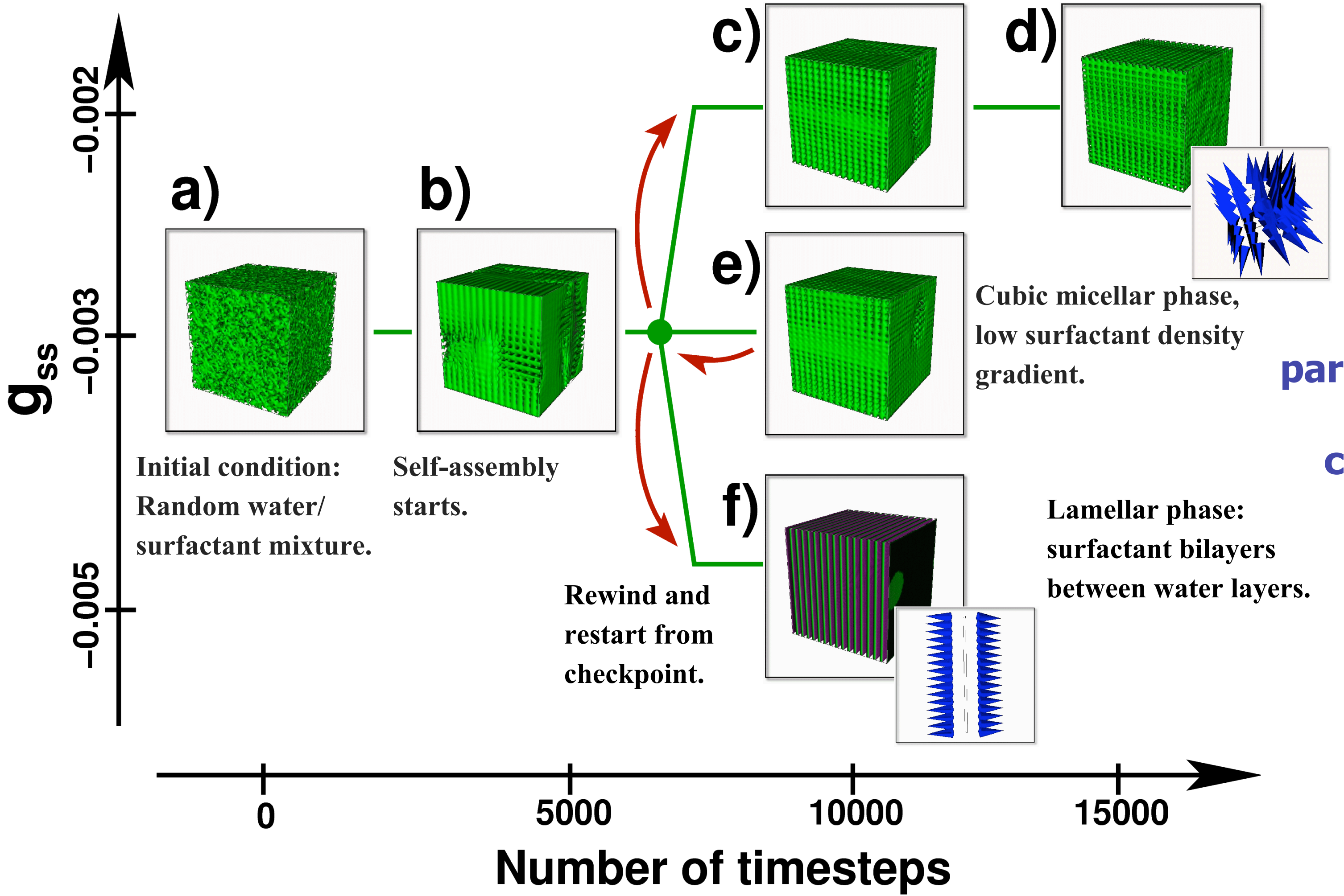
General Overview

- TeraGrid System Management & Integration Group (~40 staff)
- 9 Resource Providers (~80 staff at 9 sites)
  - Resources & Services Described via Grid "Service Level Agreements"
  - Resource: Computers, networks, instruments, databases/collections, storage systems…
- TeraGrid Architecture defines what it means to "Join TeraGrid"

How To Add a New Site: An Objective, Open Process

- Identify Resource
- Participate in Allocations Process (for compute resources)
  - Accounts, accounting processes
- Support CTSS user environment
  - Accept authentication and operation of shared coordinated software
- Participate in Operations Process
  - Define Contacts
  - Accept trouble tickets
- Join Security Infrastructure
  - Sign Security Memorandum, participate in reporting, vulnerability & risk analysis, etc.

Example use Scenario (one of many)



Initial condition: Random water/ surfactant mixture.

Self-assembly starts.

Rewind and restart from checkpoint.

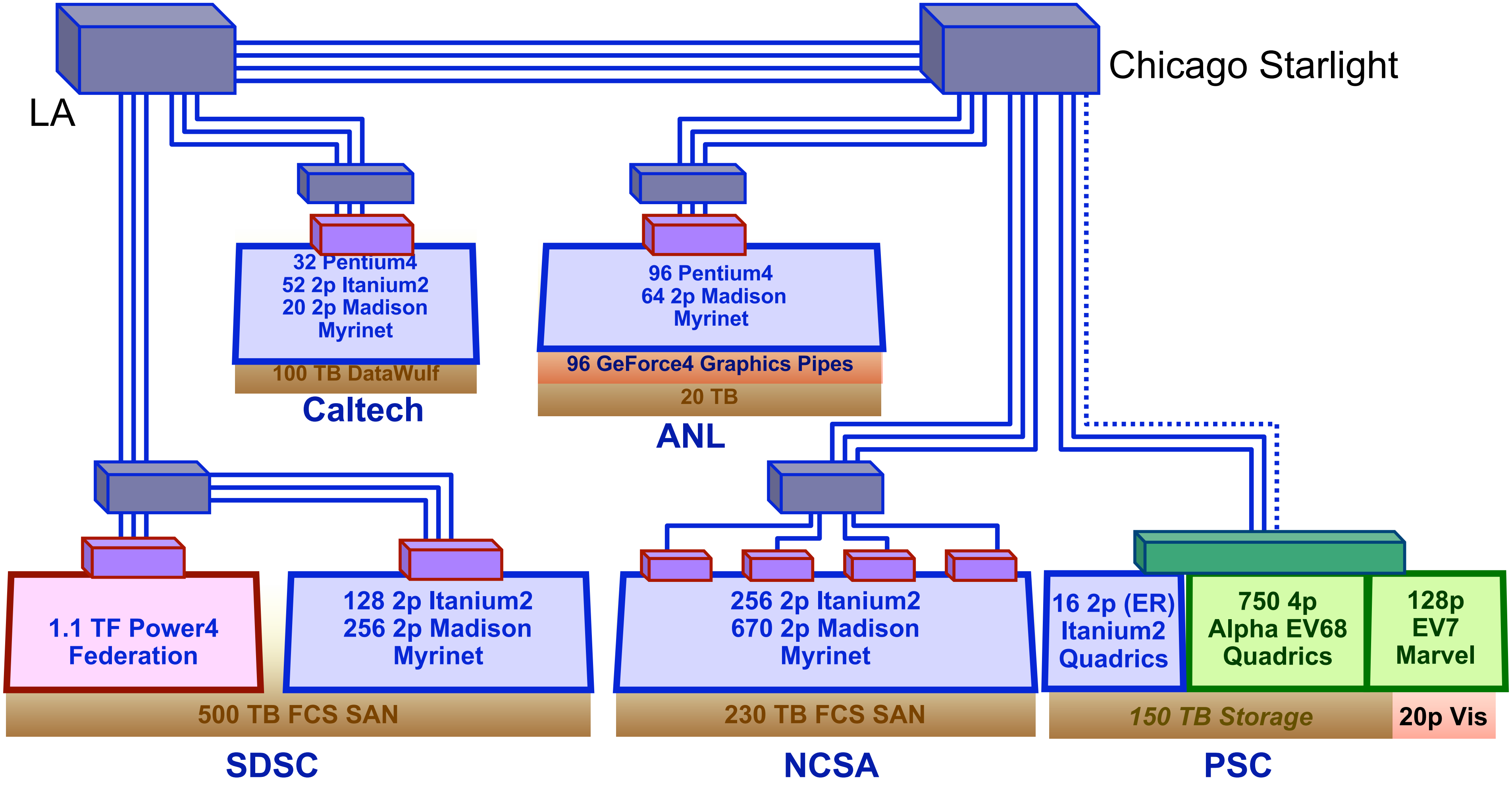
Cubic micellar phase, high surfactant density gradient.

Cubic micellar phase, low surfactant density gradient.

Lamellar phase: surfactant bilayers between water layers.

Exploring parameter space through computational steering

ETF Hardware Deployment



LA

Chicago Starlight

32 Pentium4
52 2p Itanium2
20 2p Madison
Myrinet

100 TB DataWulf

Caltech

96 Pentium4
64 2p Madison
Myrinet

96 GeForce4 Graphics Pipes

20 TB

ANL

1.1 TF Power4
Federation

128 2p Itanium2
256 2p Madison
Myrinet

500 TB FCS SAN

SDSC

256 2p Itanium2
670 2p Madison
Myrinet

230 TB FCS SAN

NCSA

16 2p (ER)
Itanium2
Quadrics

750 4p
Alpha EV68
Quadrics

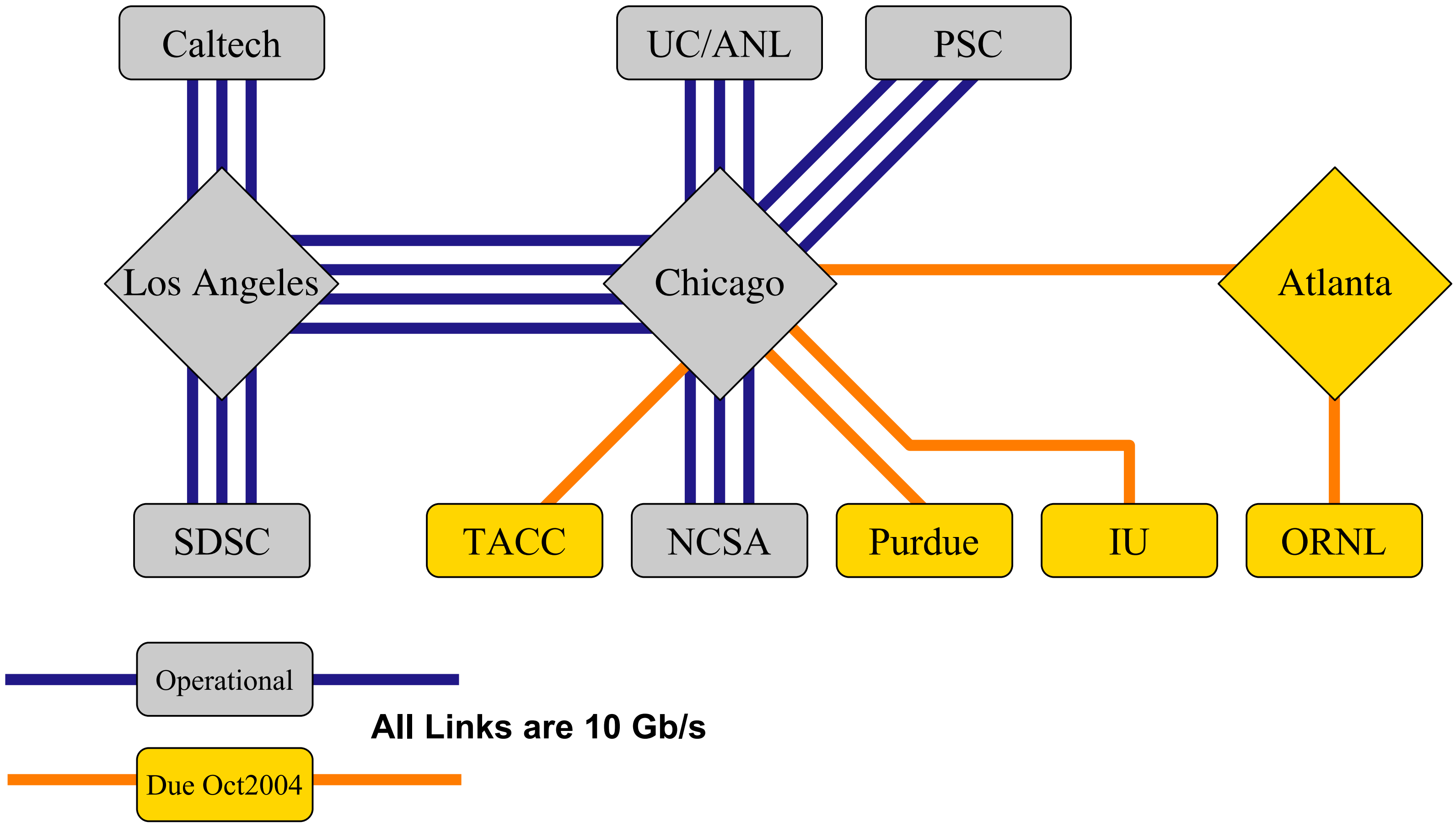
128p
EV7
Marvel

150 TB Storage

20p Vis

PSC

TeraGrid Network (June 2004)



All Links are 10 Gb/s

User-Centric Guiding Principles:

- The larger the pool of distributed, networked, ***unified*** resources, the greater the benefit
- Promoting Adoption:

Usability	**Stability**	**Capability**
It Must Be Easy	**It Must Be Ready**	**It Must Be Better**

CIO Magazine: “Timing is Everything. Seizing the perfect moment to present a new technology to your company can make or break a strategic plan.”

Unified Policies and Common Resource Currency (TROO)

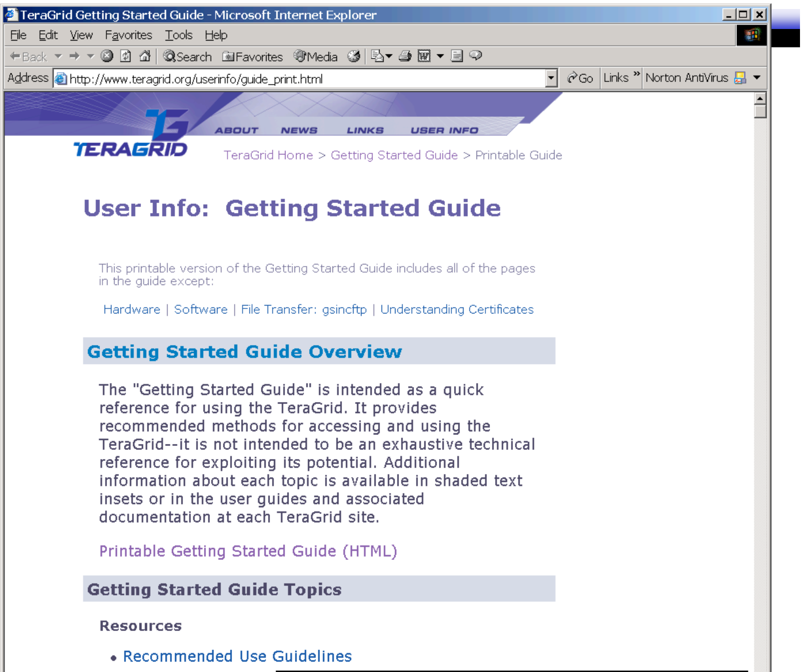
The Rule Of One

- One help desk
- One NRAC submission
- One account req. form
- One accounting currency
- One set of user policies
- One documentation set

- Result:
  - Improved Usability
  - Very attractive target for adoption
  - Unified networked resources more valuable to community (Metcalf)

Commitment To Adoption

- Learn Once, Run Anywhere (LORA)
  - A *single* training course and a *single* set of manuals preserve user investment
  - "TeraGrid Roaming" supported:
    - Develop app locally, run on any TG resource
- Result:
  - SC03 TeraGrid User Tutorial was over subscribed! Plans for road show under way
  - Smiling users
    - Improved usability & stability of TeraGrid architecture


TeraGrid Getting Started Guide - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites Media
Address http://www.teragrid.org/userinfo/guide_print.html
Go Links Norton AntiVirus
TERAGRID
ABOUT NEWS LINKS USER INFO

TeraGrid Home > Getting Started Guide > Printable Guide

User Info: Getting Started Guide

This printable version of the Getting Started Guide includes all of the pages in the guide except:

Hardware | Software | File Transfer: gsincftp | Understanding Certificates

Getting Started Guide Overview

The "Getting Started Guide" is intended as a quick reference for using the TeraGrid. It provides recommended methods for accessing and using the TeraGrid--it is not intended to be an exhaustive technical reference for exploiting its potential. Additional information about each topic is available in shaded text insets or in the user guides and associated documentation at each TeraGrid site.

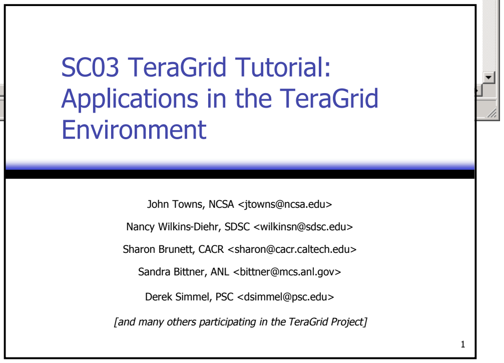
Printable Getting Started Guide (HTML)

Getting Started Guide Topics

Resources

- Recommended Use Guidelines
- Hardware
- Software Stack

Access to the Grid

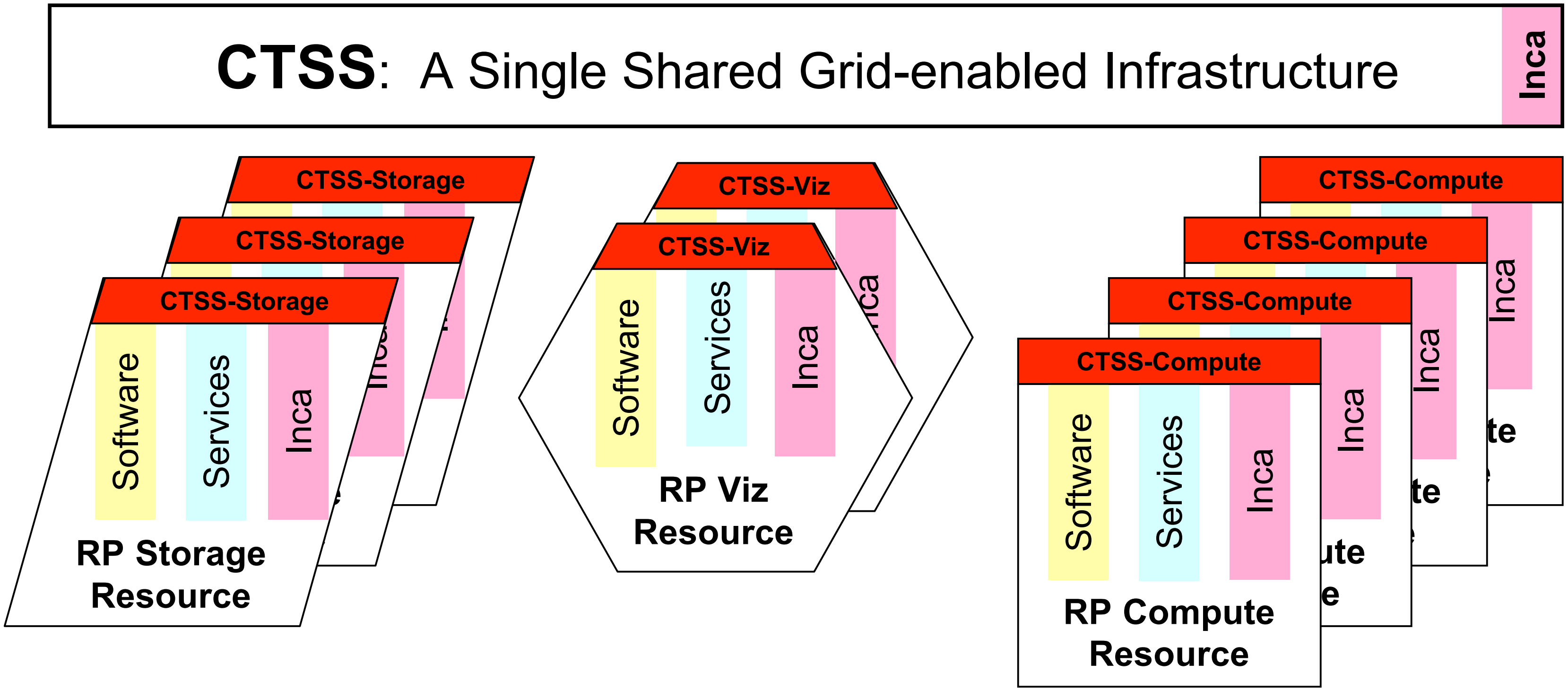


SC03 TeraGrid Tutorial: Applications in the TeraGrid Environment

John Towns, NCSA <jtowns@ncsa.edu>
Nancy Wilkins-Diehr, SDSC <wilkinsn@sdsc.edu>
Sharon Brunett, CACR <sharon@cacr.caltech.edu>
Sandra Bittner, ANL <bittner@mcs.anl.gov>
Derek Simmel, PSC <dsimmel@psc.edu>
[and many others participating in the TeraGrid Project]

1

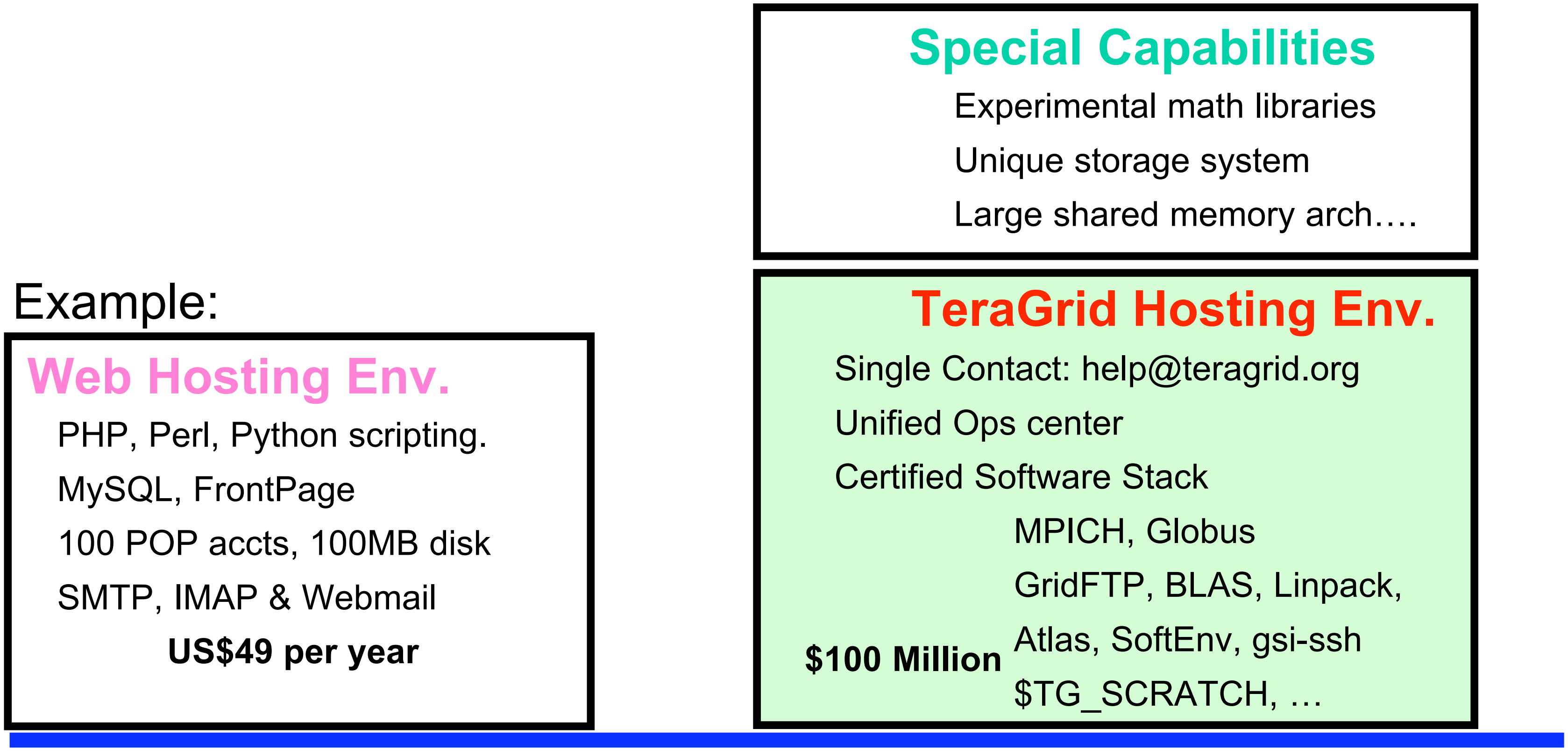
TeraGrid Architecture



Common TeraGrid Software & Services (CTSS)

A Grid Hosting Environment

The core infrastructure for Virt Orgs to build Grid-based projects



Special Capabilities

Experimental math libraries

Unique storage system

Large shared memory arch….

Example:

Web Hosting Env.

PHP, Perl, Python scripting.

MySQL, FrontPage

100 POP accts, 100MB disk

SMTP, IMAP & Webmail

US$49 per year

TeraGrid Hosting Env.

Single Contact: help@teragrid.org

Unified Ops center

Certified Software Stack

MPICH, Globus

GridFTP, BLAS, Linpack,

Atlas, SoftEnv, gsi-ssh

$TG_SCRATCH, …

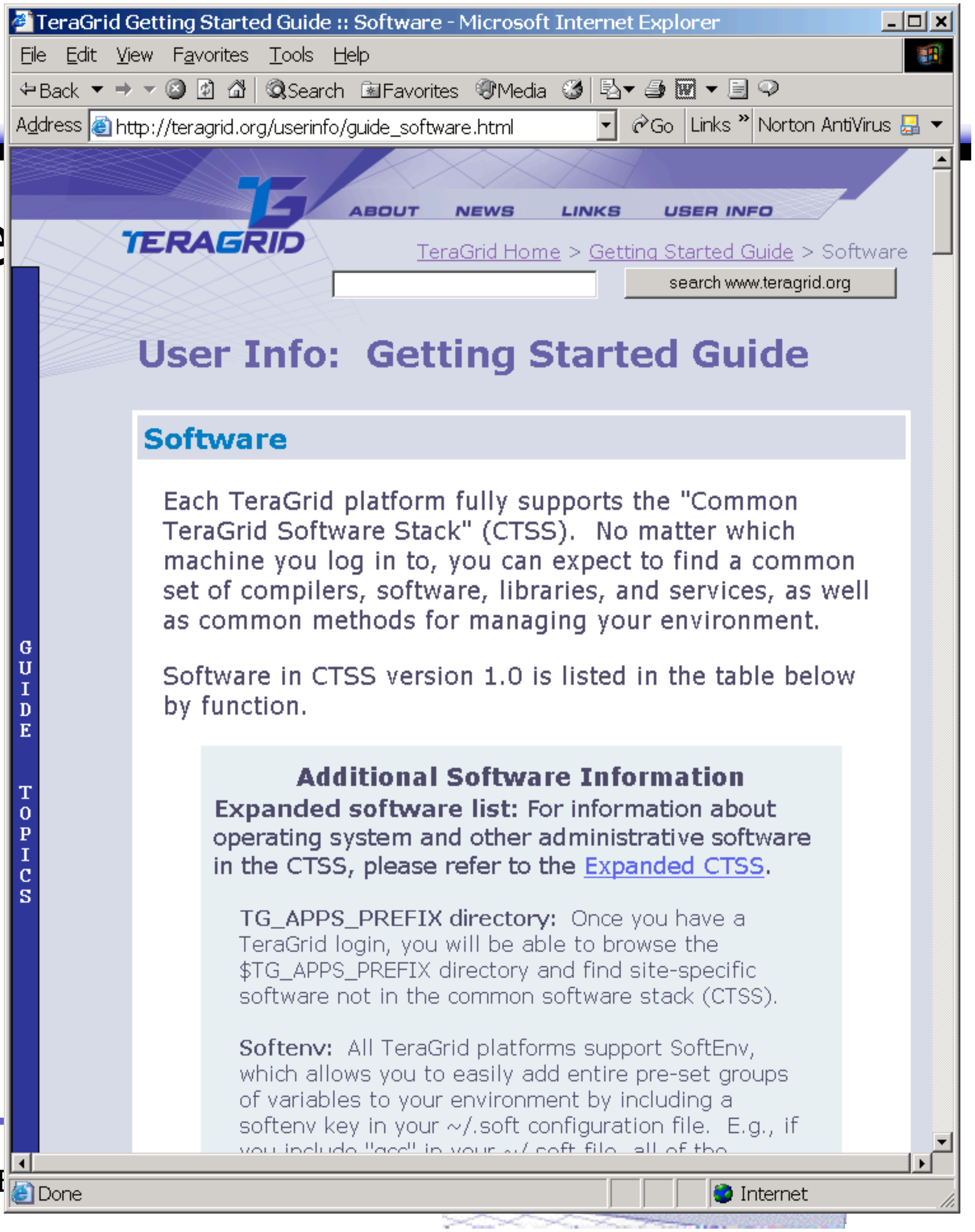
$100 Million

Classic Unix-like Environment

- /bin/sh, bin/cp, /bin/ls, Unix file system & tools, dev tools (make, compilers) etc

Common TeraGrid Software Stack

- CTSS Provides a single unified set of interoperable components and services that define the TeraGrid's Grid Hosting Enviroment and enable "TeraGrid Roaming"


TeraGrid Getting Started Guide :: Software - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites Media
Address http://teragrid.org/userinfo/guide_software.html
Go Links Norton AntiVirus
TERAGRID
ABOUT NEWS LINKS USER INFO
TeraGrid Home > Getting Started Guide > Software
search www.teragrid.org
GUIDE TOPICS
Done
Internet

User Info: Getting Started Guide

Software

Each TeraGrid platform fully supports the "Common TeraGrid Software Stack" (CTSS). No matter which machine you log in to, you can expect to find a common set of compilers, software, libraries, and services, as well as common methods for managing your environment.

Software in CTSS version 1.0 is listed in the table below by function.

Additional Software Information

Expanded software list: For information about operating system and other administrative software in the CTSS, please refer to the Expanded CTSS.

TG_APPS_PREFIX directory: Once you have a TeraGrid login, you will be able to browse the $TG_APPS_PREFIX directory and find site-specific software not in the common software stack (CTSS).

Softenv: All TeraGrid platforms support SoftEnv, which allows you to easily add entire pre-set groups of variables to your environment by including a softenv key in your ~/.soft configuration file. E.g., if you include "gcc" in your ~/.soft file, all of the

Core CTSS Components Across All Platforms: Linux, AIX, Tru64

- atlas
- blas
- condor-g
- gcc
- globus-2.2.4-gcc
- globus-2.4.3-gcc
- gsi-ncftp
- gsi-openssh
- gx-map
- hdf4
- hdf5
- Java_COG
- mpich-g2-gcc
- mpich-p4-gcc
- myproxy
- openssh
- openssl
- petsc-gcc
- python
- softenv
- srb-client
- tcl
- vmi-crm

Additional component sets, by category, include:

Intel compilers, IA64 (Myrinet, BIOS, etc), Linux kernels & patches

High Quality Production System: Integrated Verification & Validation

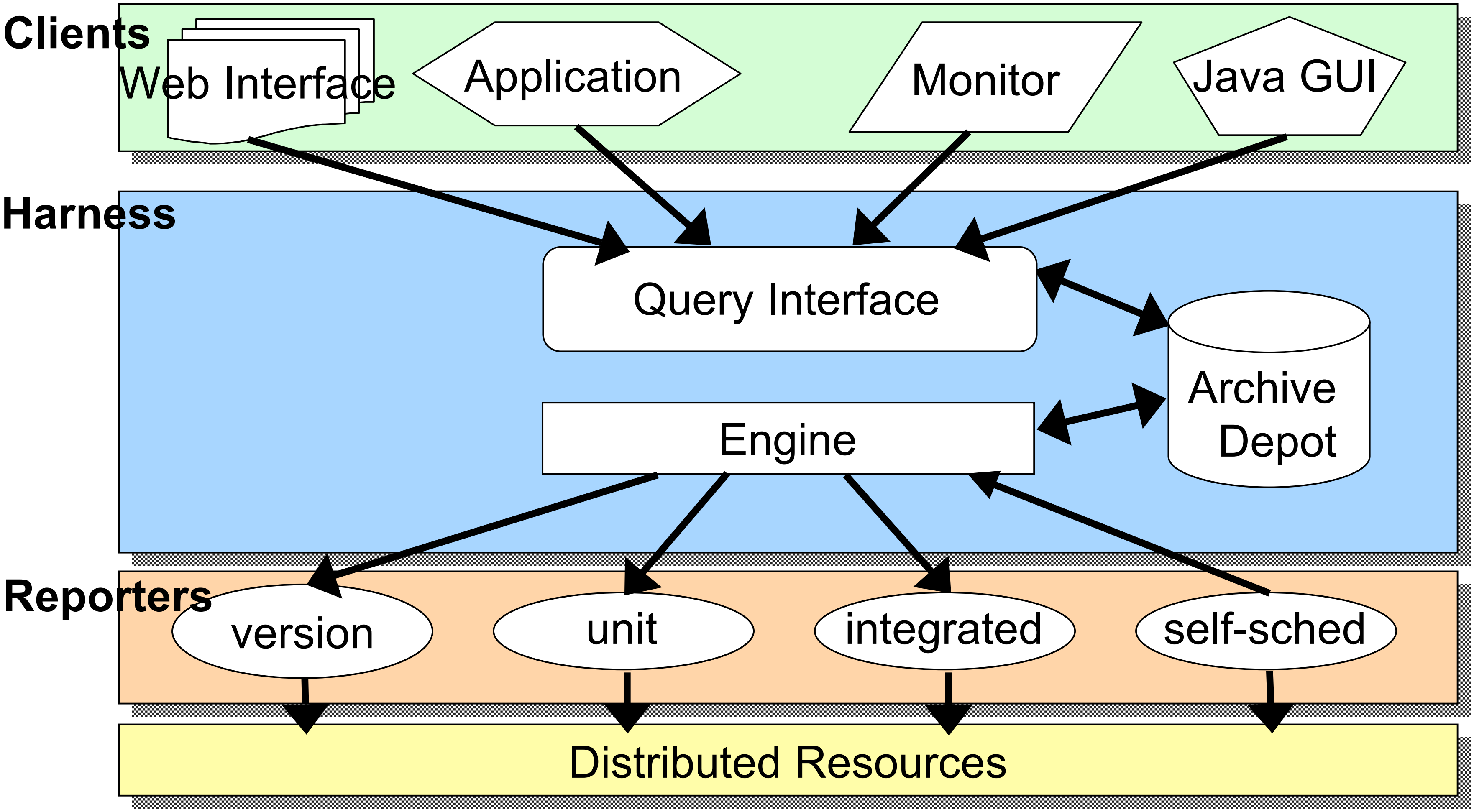
“And then one day the grid went down and never came back up.”

New Yorker Magazine, 2003

V & V Concepts for Production-Quality Grid Systems

- Formal specifications of supported environment and “operational” must exist
- A set of independent tests should check for compliance and correctness
- A human should not be “in the loop”
- Testing should include performance, and be archived over time for trend analysis
- Scalability: Adding new sites should require minimal resources

Inca: A Test Harness Framework for Builders



Source: Shava Smallen, SDSC

Across the Entire TeraGrid: A Single Language For Reporters

```
<?xml version="1.0" encoding="UTF-8" ?>  <!-- Generated by Turbo
     XML 2.3.1.100. Conforms to w3c
     http://www.w3.org/2001/XMLSchema  -->
  <xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema"
     elementFormDefault="qualified">
  <xsd:element name="INCA_Reporter">
  <xsd:complexType>
  <xsd:sequence>
  <xsd:element ref="INCA_Version" />
  <xsd:element ref="localtime" />
  <xsd:element ref="gmt" />
  <xsd:element ref="ipaddr" />
  <xsd:element ref="hostname" />
  <xsd:element ref="uname" />
  <xsd:element ref="url" />
  <xsd:element ref="name" />
  <xsd:element ref="description" />
  <xsd:element ref="version" />
  <xsd:element ref="INCA_Input" />
  <xsd:element ref="body" />
  <xsd:element ref="exit_status" />
  </xsd:sequence>
  </xsd:complexType>
  </xsd:element>
  <xsd:element name="gmt" type="xsd:string" />
  <xsd:element name="localtime" type="xsd:string" />
  <xsd:element name="hostname" type="xsd:string" />
  <xsd:element name="ipaddr" type="xsd:string" />
  <xsd:element name="uname" type="xsd:string" />
  <xsd:element name="url" type="xsd:string" />
  <xsd:element name="name" type="xsd:string" />
  <xsd:element name="version" type="xsd:string" />
  <xsd:element name="INCA_Version" type="xsd:string" />
```

```
<xsd:element name="description" type="xsd:string" />
<xsd:element name="exit_status" nillable="true" fixed="0">
<xsd:complexType mixed="true">
<xsd:choice>
<xsd:element ref="message" minOccurs="0" />
</xsd:choice>
</xsd:complexType>
</xsd:element>
<xsd:element name="message" type="xsd:string" />
<xsd:element name="body" abstract="true" />
<xsd:element name="ID" type="xsd:string" />
<xsd:element name="INCA_Input">
<xsd:complexType>
<xsd:sequence>
<xsd:element ref="input" minOccurs="0" maxOccurs="unbounded" />
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="input" />
<xsd:element name="verbose" type="xsd:integer"
    substitutionGroup="input" />
<xsd:element name="help" substitutionGroup="input">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="yes" />
<xsd:enumeration value="no" />
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
</xsd:schema>
```

Current Status of V&V Program

- More than 900 components are tested
- Output is “engineer quality”, and not prioritized or user readable
- Definition of “Up” underway
- Inca has been well received by other Grid communities, and we are beginning to receive requests for copies and presentations

In Practice…