TeraGrid’s Integrated Information Service “IIS”

Grid Computing Environments 2009


TeraGrid Grid Infrastructure Group (GIG)
University of Chicago, Argonne National Laboratory

November 2009
Introduction:
Conceived in 2006; Production in 2007; Presented at GCE’07.
IIS Vision

1st IIS System Architecture
Distributed CI provider operated local information services
Centralized federation wide information services
Registries -> XML document entries

2nd IIS Information Architecture
Registry architecture and data format
The Capability Kit meta-registry
Current information registries

Leveraging IIS Examples – Providers and Consumers

Conclusion and Future Work

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Vision

Provide an **Authoritative Integrated Information Service** enabling:

Human discovery of cyber-infrastructure

- Science Gateways, Portals, Documentation, CLIs

Software discovery of cyber-infrastructure

- For automated resource, service, and software selection and access
- For auto-configuration (applications, gateways, workflow engines)

Providers to advertise their cyber-infrastructure offerings

- Advertise any information about any CI capability
- Providers own data, and independently control publishing

Streamlined operations

- Change integration and management
- Automated testing, and monitoring

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Provide an Authoritative Integrated Information Service enabling:

- Human discovery of cyber-infrastructure (Science Gateways, Portals, Documentation, CLIs)
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Distributed Architecture Components

Federation Wide
Integrated Information Service

Service Provider
Local Information Service

TeraGrid
Wide Databases

XML Repository

Apache 2.0

Tomcat
WebMDS

WS MDS4

WS/REST

WS/SOAP

Clients

Clients

HTTPD

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High-Availability Architecture

Service Provider Publishing

High-Level Aggregation

Clients

info.teragrid.org

Dynamic DNS
Information Architecture

Registry Architecture
Named Registries, with schema compliant
Registry Entries, which are each an
XML Document

The Capability Deployment Meta-Registry

Universal Identifiers
Site and Resource Identifiers
Capability Identifier
Registry entry cross-references

Extensibility
Meta-Registry Extensions
New Registries
XML
TeraGrid Capability Meta-Registry

Each Capability Deployment
Where (site and resource)
What (name, class, and description)
Support information
Status information
Software and services component information
Extensions

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Capabilities Kit Registry by Class

**CTSS**
- Application Development & Runtime
- TeraGrid Core Integration (local info service)
- Co-scheduling, meta-scheduling
  - *Common Client*
  - *Computation & Scheduling Clients*
  - *Data Collections*
  - Data Management
  - Data Movement servers, Clients
  - Distributed Parallel Application Support
  - *Distributed Programming Systems*
  - *Local Compute*
  - Login
  - *Nimbus/Cloud Computing*
  - Parallel Application Support
  - Remote Computation
  - Science Gateway Support
  - Visualization Software (VTSS)
  - WAN GPFS, WAN Lustre file-systems
  - Workflow Support

**Gateways**
- *Renci Portal*
  - *

**Local**
- Local HPC Software

**Central**
- *Credential Server (MyProxy)*
- *Integrated Information Services*
- *User Portal*
Other Registries

Gateways Registries

*Science Gateway Web Services Application Registry*

CTSS Extension Registries

- Batch System Load (%)
- Batch Queue Contents (requires authorization)
- OGF GLUE2

Local RP Registries

*Local HPC Software Catalog*

TeraGrid Central Database Registries

- Site/Organization and Resource identifiers (IDs) and descriptions
- Project/Allocation to Resource authorization list
- TeraGrid Science Gateway Catalog
- *TeraGrid System Outages*
Leveraging IIS Examples

Resource Description Repository Publishing

TeraGrid User Portal Batch Load & Queue Data
TeraGrid User Documentation

Software Discovery
- CTSS Software
- Local HPC Software
- Science Gateway Software
- Science Gateways Web Services “WS” Application Registry

Advanced Scheduling Information

Inca Verification & Validation
User Profile Service
Discovery CLI Interface

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TeraGrid Core Services uses RDR to collect and store validated, current and historical resource description information:

- Common Resource Information
- Compute Resource Information
- Data Collections Information
- Storage Information
IIS provides queue & batch load information from all RP sites for TGUP to use in system monitor.
http://www.teragrid.org/
http://www.teragrid.org/userinfo/software/ctss.php
Software Discovery

TeraGrid context:
> 650 CTSS software package deployments
> 1600 Local HPC software package deployments
> 40 Science Gateways offering software packages

Problems:
How can users discover what software is available, and how to access it?
How can Science Gateways or Web Applications discover what software is available thru web service interfaces and invoke it?
Software Discovery

Solutions:

- Single IIS interface to multiple software repositories including 3rd party HPC software and Science Gateway software.
- A custom Gateway web services registry.

Which enables, for example:

- Scientists to discover that Gaussian is available both from the command line and through a full service gateway such as GridChem (www.gridchem.org).
- Science Gateways and Applications to discover and invoke Gaussian web services automatically.
Software Discovery Design

Kit Registry
- CTSS Kit Software
- Gateways Kit Software
- Local HPC Kit Software

Comprehensive Software Discovery

WS Enabled Software Discovery

Local HPC Software Registry

Gateway Web Services Registry

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Each Gateway hosts a service (RESTful or otherwise) that publishes local web service metadata.

Information Services aggregates all configured Gateway hosted GAWSR metadata, creating a central registry.

Content of GAWSR metadata is rich enough to dynamically launch jobs via web services. (ie, the registry has enough metadata to allow a user/client to dynamically launch jobs)

Following slides demonstrate two clients using the GAWSR. The first & the latter is a.
Dynamic execution of web services written in Java
RIA Flex application showing the available metadata

**Web Service Info**
- **Name:** Blast
- **Executable:** blastall
- **Science Bundle:** NCBI (2.2.18)
- **Description:** Comparison of nucleotide or protein sequences from organisms

**Required Inputs**

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<tr>
<th>Name</th>
<th>Flag</th>
<th>Type</th>
<th>Default Value</th>
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<td>believe</td>
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<td>f</td>
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<td>show_gi</td>
<td>-i</td>
<td>CHECKBOX</td>
<td>f</td>
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<tr>
<td>view_alignments</td>
<td>-m</td>
<td>SELECT</td>
<td>7</td>
</tr>
</tbody>
</table>

**Optional Inputs**

**Accessor Info**
Local HPC Software

SiteID: iu.teragrid.org
ResourceID: bigred.iu.teragrid.org

Software:
- AMBER - 9.0 - Molecular mechanics & dynamics packages
- ant - 1.6.5 -
- ATLAS - 3.6.0 - Automatically Tuned Linear Algebra Software
- BLACS - MPICH-MX version - Basic linear algebra comm subprogram
- BLAST - 2.2.26 - Biology Database Search tool
- BOXSHADE - 3.31 - Program for pretty-printing multiple alignment output.
- CDO - CDO 1.0.7 - Command line Operators to manipulate and analyse Climate Model Data
- Chaco - 2.2 - Multilevel graph partitioning package
- CHARMM (Harvard Version) - c12b1 - General purpose molecular modeling pigs
- CLEPP - 1.9.3-1.1, X11 build - Class library for High Energy Physics Description
- CLISP - 2.41 - Common Lisp, abbreviated as Cl, is a dialect of the Lisp programming.
- ClustalW - MPI-1.14 - Fully automatic program for global multiple alignment of DNA
- cmake - 2.4.7 - CMake, the cross-platform, open-source make system
- condor - 6.9.3-r1 - Condor is a specialized workload management system for compute-intensive jobs
- CPMD - 3.1, IBM-64 - Car-Parrinello Molecular Dynamics
- CVS - 1.11.14 - version control system
- DOCK - 5.4 - problem of binding molecules to each other
- FASTA - 33 - DNA and Protein sequence alignment software
- FFTW - 2.1.3 and 3.0 - Routines for discrete Fourier transforms
- GAMESS - Ab initio quantum chem (wavefunctions)
- GARLI - 0942-IBM-mpich-32 - Heuristic phylogenetic package using GTR model
- Gaussian 03 -

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Advanced Scheduling Information

CTSS
- Co-scheduling
- Meta-scheduling
- Computation & Scheduling Clients
- Local Compute
- Remote Computation
- Science Gateway Support
- Workflow Support

GLUE2 Registry
Inca Verification & Validation

- Running on TeraGrid since 2003
- Verifies IIS published information through automated, user-level testing
- Total of ~2200 tests running on 18 login nodes, 2 grid nodes, and 3 servers
- Email notifications for critical services
- Status views from detailed test information to summary and historical reports
- Data published as XML, HTML, or graphed
- IIS compatible REST interface:
  - http://info.teragrid.org/
  - http://inca.teragrid.org/
User Profile Service

Provide authenticated users with user-centric information
HTTPS with Basic Authentication
In html, csv, json, perl, and xml formats

Web Application profile-v1 Usage

Supported URLs
https://info.teragrid.org:8444/web-apps/html/profile-v1/project/project_number/$project_number/
https://info.teragrid.org:8444/web-apps/html/profile-v1/project/project_number/$project_number/job/
https://info.teragrid.org:8444/web-apps/html/profile-v1/project/project_number/$project_number/collab/

Description
Profile information for the authenticated user
All users with which the authenticated user shares a project
12 month job history for the authenticated user
Project information for the given project of the authenticated user
Job history for the given project of the authenticated user
Collaborators of the authenticated user for the given project
Job history for the authenticated user with the given allocation on the given resource
Resource information for the authenticated user
Resource information for the authenticated user's given resource
Job history for the authenticated user on the given resource
Job history for the authenticated user with the given allocation on the given resource
This usage page
Discovery CLI Interface

The tginfo CLI:  http://info.teragrid.org/tginfo/

![Terminal screen showing tginfo res and software hdf5]

### TGInfo res

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<thead>
<tr>
<th>ResourceID</th>
<th>ResourceName</th>
<th>Type</th>
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<tr>
<td>bigben.psc.teragrid.org</td>
<td>bigben.psc.teragrid.org</td>
<td>Compute</td>
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<tr>
<td>cobalt.ncsa.teragrid.org</td>
<td>NCSA Cobalt Altix</td>
<td>Compute</td>
</tr>
<tr>
<td>lincoln.ncsa.teragrid.org</td>
<td>NCSA Lincoln</td>
<td>Compute</td>
</tr>
<tr>
<td>spur.tacc.teragrid.org</td>
<td>TACC Spur</td>
<td>Compute</td>
</tr>
<tr>
<td>condor.purdue.teragrid.org</td>
<td>Purdue Condor Pools</td>
<td>Compute</td>
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<td>queenbee.loni-lsu.teragrid.org</td>
<td>LONI QueenBee</td>
<td>Compute</td>
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<td>ranger.tacc.teragrid.org</td>
<td>TACC Ranger</td>
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<td>brutus.purdue.teragrid.org</td>
<td>Purdue Brutus (FPGA)</td>
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<td>dtf.ncsa.teragrid.org</td>
<td>NCSA DTF Mercury</td>
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<td>bigred.iu.teragrid.org</td>
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<td>steele.purdue.teragrid.org</td>
<td>Purdue Steele</td>
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<td>kraken.nics.teragrid.org</td>
<td>NICS Kraken Cray XT5</td>
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### TGInfo software hdf5

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</table>
Conclusion

Federation Wide Standards
- Information Integration Identifiers
- Information Discovery REST APIs
- Standard Capability Naming and Description Schemas

Federation Wide Information Discovery
- Using a Central Federation Wide Index
- Using a DNS/WWW model
- Central Discovery → Distributed Information Access

Enable User Interfaces
- Web 2.0, Science Gateways, and traditional Web servers
- ** IIS does not develop those interface
Conclusion & Future Work

Information Architecture

- Capability Definition Meta-Registry (BioMedical Informatics -- BIRN)
- Capability Implementation Registry
- More Capabilities and Capability Classes
  Clouds/IaaS, SaaS, Distributed Programming Environments (SAGA), Data Collections
- Science Gateway Security Configuration Information (SAML)

System Architecture

- Fully REST based registration services (Apache CXF, Globus CRUX)
- Fully REST based aggregation services
- More REST based discovery interfaces (with XPATH, XSLT support)
- More custom REST service, some providing custom user services

Separate IIS project

- Packaged, documented, and distributed for other projects

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More Information

Web Sites
- http://info.teragrid.org/
- http://www.teragrid.org/gateways/
- http://info.teragrid.org/web-apps/html/index/ (REST APIs)

People
- JP Navarro, Lee Liming (IIS Architecture and Coordination)
- Nancy Wilkins-Diehr (Gateway Information)
- Warren Smith (Execution and Scheduling Information)
- Ed Hannah (Resource Description Information)
- Kate Ericson (Monitoring and Validation Information)
- Rion Dooley (Authenticated User Custom Information)