Scientific Computing with UNICORE

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Outline

- Introduction
- Grid Computing Concepts
- Unicore Architecture
- Unicore Capabilities
- Unicore – Globus Interoperability
- Summary
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Uniform Interface to Computer Resources

- conceived in 1997 by German universities
- expanded in UNCICORE-Plus (2002), EUROGRID, GRIP, OpenMolGRID
- designed to provide users with seamless, secure and intuitive access to heterogeneous computing resources
- acts like a client that provides a grid infrastructure and gives access to selected Globus resources allowing job submission, status queries, data staging, and output retrieval.
UNICORE system

- servers run on Unix systems (IBM AIX, Sun Solaris, SGI Irix, Linux) supporting Java 1.3 (2)
- Interfaces for batch systems on CLAY, SGI, SUN, Fujitsu, IBM, NEC, Hitachi, Siemens
- IBM’s Load Leveler, PBS, PBS Pro
Grid Computing concepts

- facilitate users interaction with advanced problem-solving tools
- resources and individual might be part of multiple Grid
- authentication and authorizations - security
- resource management - integration of resources and exposure of related services
- users, applications and higher-level services must be able to find appropriate resource candidates
Unicore Architecture

Three tier architecture:
- User (Client)
- Server
- Target system

Security model:
- X.509 certificate
- SSL
Unicore Architecture- User

- **Unicore Client** – a Java GUI to exploit the server’s functionality:
  - creation, manipulation and jobs submission
  - job monitoring and control
  - management of user’s security
  - login and debug information

- Uses *Job Preparation Agent* (JPA) to create jobs, adds the client’s certificate and sends it to server (*Gateway*) as *Abstract Job Object* (AJO)
Unicore Architecture - Server

• The Gateway and Network Job Supervisor (NJS) are executed on dedicated secure systems, behind a firewall

• Gateway authenticates the user and transfers the AJO to the NJS

• The Network Job Supervisor translates AJO into a target system specific batch job using Incarnation Database (IDB)
• *Target System Interface (TSI)* is a daemon executed on the target system.

• *TSI* interfaces the local operating system with the local batch subsystem
Unicore Capabilities

- Uspace is a temporary data space - working directory for running jobs on Usite
- all functions necessary to move data between Uspace and the client (controlled by client)
- data movement between Uspace and file systems at Vsite is specified by user or by application
- data transfer between Usites is controlled by NJS
- data transfer by a byte streaming protocol or within an AJO for small data sets
- Alternative File Transfer (AFT) mechanism based on GridFTP – ability to transfer file between two target systems
Unicore Capabilities

Security
- certificates according X.509 standard
- all grid members should use the same certificate authority (CA) for both user and server certificates.

Execution Mgmt
- UNICORE relies on descriptions of resources available at run job creation and submission time to the client
- Global Grid Forum imposed standards on Grid Information Services, Scheduling and Resource Management.

User’s Perspective
- There are software packages like Gaussian, Car Parrinello Molecular Dynamics, Fluent accessible with UNICORE, which address:
  - Chemists and bio-molecular scientists
  - Meteorological scientists
  - Scientific users of coupled HPC applications
Unicore Capabilities

Quantum Mechanic Package Gaussian 98

Figure 3. Gaussian plugin and output Visualization
Unicore Capabilities

Amber Package of Molecular Simulation Programs

Figure 4. Amber plugin: Input preparation wizard.

Figure 5. Amber plugin: Help.
Unicore Capabilities

Protein DataBase (PDB) search plugin

Figure 6. PDB Search plugin.

Figure 7. Output visualization.
Unicore Capabilities

New version of Local Model - meteorology

Figure 8. Meteo plugin.

Figure 9. Forecast visualization.
Unicore – Globus Interoperability

Key Points

• Translating UNICORE requests for job submission, output retrieval and status queries to the corresponding Globus constructs

• Mapping of permanent UNICORE user certificates to temporary Globus proxy certificate

• Implementation without change in architecture
Enhanced Target System Interface (ETSI)

• UNICORE handles it as one of the target systems
• Globus as a client application using standard API
Unicore – Globus Interoperability

Solution

• The *Proxy Certification Authority (Proxy-CA)* was developed

• *Proxy-CA* is integrated into the Enhanced TSI by the *Certification Authority Interface (CAI)* component

• The Enhanced TSI is implemented in C and Perl
Summary

- UNICORE-Globus interoperability demonstrated the feasibility of Grid interoperability – they can be combined successfully.
- Jobs can be submitted to Globus system from UNICORE client and the results are returned to the user.
- Extends the resources available to UNICORE.
- Provides Globus users with a graphical job-submission interface.
References and Further Readings

• Dirk Breuer, Dietmar Erwin & all, “Scientific Computing with UNICORE”
• Dietmar Erwin, “UNICORE – A Grid Computing Environment”
• Ian Foster, Carl Kesselman, “The Grid: Blueprint of a New Computing Infrastructure”
• Michael Rambadt, Philipp Wieder, “UNICORE-Globus: Interoperability of Grid Infrastructure”
• “UNICORE Forum”, http://www.unicore.org
• D. Snelling, “UNICORE and the Open Grid Services Architecture”
• “The Portable Batch System”, http://www.openpbs.org

Thank you!