Status and Future of European GRID Development

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Outline

- UNICORE approach
- UNICORE architecture and implementation
- UNICORE projects
- Availability and outlook
- UNICORE and OGSA
- Pallas company profile

UNICORE Approach

- Provide a seamless work environment for end-users
  - uniform access and authentication mechanism
  - hide execution system details
  - offer user-level resource and workflow model
- Support end-users in specific science/engineering domains
  - support important applications
- Emphasize security
  - site security
  - data and workflow integrity
- Preserve autonomy of participating sites
  - firewalls and security policy
  - system administration,
  - user administration and accounting
- Designed for production use

UNICORE History

- Started as a seamless access platform for German HPC centers
  - project UNICORE (1997–1999)
    ⇒ UNICORE Grid phased into operation in 2003
- Embracing the Grid philosophy, enhancing functionality
  - project EUROGRID (IST–1999–20247)
    ⇒ dynamic resource identification and brokering
    ⇒ plugins provide user-friendly interfaces
- Introducing compatibility to Globus
  - project GRIP (IST–2001–32297)
    ⇒ combine EUROGRID and Globus resources
    ⇒ pave the way towards OGSA

UNICORE Functionality and Services

- Access grids securely
- Construct workflows
- Submit to computing resources
UNICORE Functionality and Services

- Monitor progress, retrieve results
- Control & steer execution

UNICORE Functionality and Services

- Application-specific interfaces

UNICORE Resource Model

- UNICORE site(s)
- Virtual site(s)
- User submits jobs to a Vsite – soon: automatic resource identification
- Resources – capacity – capability
- Resources are advertised to the client – pseudo-dynamic mode

UNICORE Job Model

- Directed acyclic graph of
  - tasks (computational or data transfer)
  - sub-jobs (to be executed at another Vsite)
  - temporal dependencies
- Attach resource requests to tasks
  - capacity (CPU time, disk, ...)
  - capability (MPI–2, profiling, ...)
  - can do static tests of jobs
  - can do resource brokering ...

UNICORE Architecture

- Client can run anywhere
- Gateway as single point of entry
- NJS incarnates and schedules jobs
- UDB (User Database) contains user login information
- IDB (Incarnation Database) contains resource information and job incarnation rules
- TSI (Target System Interface) interfaces to local batch system

UNICORE Security Model

- User authentication
  - Gateway requires user certificate to initiate SSL communication
  - pass (permanent) user certificate along with job description
  - can pass site-specific authentication information (e.g. SecurID passcode)
- User authorization
  - Vsite maps certificate to local userid
  - authorization based on local userid
- Workflow integrity
  - each DAG is signed with the private key
  - the Vsite executing a sub-job can check the sign
- Trust model
  - require the user to protect his/her private key
  - require the CA to be safe
  - don’t require transitive trust between sites!
UNICORE Technology

Client and server components implemented in Java–2

Authentication uses X.509 certificates
  – software can work with any PKI scheme
  – even Globus temporary certificates can work ...

Coexistence with firewalls
  – gateway as single point of entry
  – can run outside firewall, in DMZ or inside firewall
  – user authentication at that point: rogue users can’t go further

Secure data transmission using SSL
  – additional data encryption considered in EUROGRID

Use of XML for
  – storing workflows
  – databases

UNICORE GUI – Authentication

Unlock keystores

CA certificate

User certificate

UNICORE GUI – Main Screen

Job panel

Main dialog area

Action buttons

Monitor panel

UNICORE GUI – Job Construction

Task graph

Available sites

Available machines

UNICORE GUI – Task Definition

Job structure

Script text

Files to be imported

Files to be exported

UNICORE GUI – Specify Resources

Software resources

Resource limits

Check values

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UNICORE GUI – Export Files

- File to be exported
- Destination
- Name at destination
- Directory browser
- List of all exports

UNICORE GUI – Run a Job

- Refresh action button
- Job and task status

UNICORE GUI – Look at Job Output

- Task stdout
- Retrieve output
- Task stderr

Application Frontends

- Create GUIs that support important applications
  - UNICORE client has a plugin interface
  - GUI simplifies data entry for application
  - GUI can support application-specific resources
  - GUI constructs (complicated) job chains automatically
- GUI will use UNICORE client to
  - submit the application job
  - monitor and control the application job
- Helpful features
  - end-users concentrate on applications
  - extended consistency checks
- Existing frontends
  - CPMD molecular dynamics code
  - Fluent, Gaussian, ...

Projects Around UNICORE

UNICORE = GRID system for seamless access to (High Performance) Computing Systems

<table>
<thead>
<tr>
<th>Project</th>
<th>Goals</th>
<th>Duration</th>
<th>Funded by</th>
</tr>
</thead>
<tbody>
<tr>
<td>UNICORE Plus</td>
<td>Product, Deployment at HPC Centers</td>
<td>01/2000 - 12/2002</td>
<td>Germangovt.(BMBF)</td>
</tr>
<tr>
<td>EUROGRID</td>
<td>European HPC centers, scientific applications, industrial involvement</td>
<td>11/2000 – 10/2003</td>
<td>EU FP5</td>
</tr>
<tr>
<td>GRIP</td>
<td>Interoperability UNICORE and GLOBUS</td>
<td>01/2002 – 12/2003</td>
<td>EU FP5</td>
</tr>
<tr>
<td>Various new projects</td>
<td>Applications, tools, deployment, ...</td>
<td>≥ 2002</td>
<td>EU FP5/FPP</td>
</tr>
</tbody>
</table>

UNICORE Plus Project

- German national R&D project
- Production version (4.0) available since August 2002
- Current phase: production deployment
- Involvement of major German HPC centers
  - FZ Jülich
  - LRZ München
  - ZIB Berlin
  - PCT Paderborn
  - HLRS Stuttgart
  - RZ Karlsruhe
  - DWD
- Involvement of vendors
  - Cray/SGI
  - Hitachi
  - IBM
  - Siemens
  - Fujitsu
  - HP
  - NEC
  - Sun
- Involvement of ISVs
  - Pallas
  - Fujitsu Labs Europe
EUROGRID – UNICORE in Europe

- Started end of 2000
- Based on UNICORE software release 3.0/4.0
- Domain-specific Grids and extensions
  - biology, meteorology, CAE
- General-purpose extensions
  - data transfer, resource brokering, ASP, interactive use
- Current phase: Grids operational, prototypes available

Involvement of European HPC centers
- FZ Jülich
- CNRS-IDRIS
- DWD
- University of Manchester
- Parallab
- ICM Warsaw
- CSCS

Involvement of industry
- EADS CCR
- debis Systemhaus
- Pallas
- ICM Warsaw
- Univ Bergen (N)
- Univ Manchester (UK)

EUROGRID Partners

HPC Centers
- CSCS Manno (CH)
- FZ Jülich (D)
- ICM Warsaw (PL)
- IDRIS Paris (F)
- Univ Bergen (N)
- Univ Manchester (UK)

Users
- Deutscher Wetterdienst
- EADS
- debis Systemhaus (Assistant Partner)

Integration
- Pallas (Project Coordinator)
- Fecit (Assistant Partner)

Volume: 33 person years, 2 MEuro funding by European Commission Grant No. IST–1999–20247

Bio–GRID – Towards a Bio–Molecular PSE

- Operate a GRID for bio–molecular simulations
- Create a bio–molecular PSE
- Integrate existing biological and chemical codes

CAE–GRID – Coupled Simulations

- Run coupled aerospace simulations (structure & electromagnetism)
- Use CORBA as coupling substrate
- Provide internal portal for EADS engineers

EUROGRID – On–Demand Prediction

On–demand mesoscale weather prediction system
- Based on relocatable version of DWD’s prediction model
- Works from regular prediction data, topography and soil database

Meteo–GRID – On–Demand Prediction

User

EUROGRID node

DWD

GME2LM

Interpolation of GME results to LM grid

1 - 5 MByte

Topographical data set

50 MByte

Initial and lateral boundary data sets on GME grid

LM

Calculation of weather forecast

LM-forecast data

Visualisation

~50 MByte

50 - 100 MByte

Initial and hourly lateral boundary data sets on LM grid (1 - 20 GByte)

LM-forecast data

Visualisation

~50 MByte
CAE–GRID – ASP for Engineering Applications

- Integrate mechanisms for cost prediction, accounting and billing
- Build HPC portal for engineers and standard CAE applications (Nastran, Fluent, ...)
- Cooperation with T–Systems (leading industrial HPC provider)

EUROGRID Technology

- Based on UNICORE system
- Develop additional GRID components
  - efficient data transfer
  - ASP infrastructure
  - resource broker
  - application coupling
  - interactive access
- Integration of new components by Pallas and Feclt

GRIP Partners

<table>
<thead>
<tr>
<th>HPC Centers</th>
<th>Users</th>
</tr>
</thead>
<tbody>
<tr>
<td>FZ Jülich (D, Coordinator)</td>
<td>ICM Warsaw (PL)</td>
</tr>
<tr>
<td>Univ. Manchester (UK)</td>
<td>Deutscher Wetterdienst</td>
</tr>
<tr>
<td>Univ. Southampton</td>
<td></td>
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</tbody>
</table>

Volume: 18 person years, 1.2 MEuro funding by European Commission Grant No. IST–2001–32257

GRIP – Compatibility to Globus

- Started as IST project beginning of 2002
- Develop interoperability software for
  - using Globus resources from UNICORE
  - transparent brokering of Globus and UNICORE resources
- evaluate the interoperability with
  - biomolecular applications from ICM
  - on-demand weather prediction from DWD
- To move the UNICORE software towards OGSA

GRIP – Interoperability Architecture

- UNICORE components
- Interoperability components
- Globus components

- FZJ
- Argonne National Labs
- ICM Warsaw (PL)
- Deutscher Wetterdienst
- Pallas
The UNICORE Forum

- UNICORE Forum owns IPR in UNICORE architecture
- Established as Association (under German law)
- Membership open for everybody (organization or persons) interested in Grid technology
- Currently ≈ 28 members (HPC centers, hardware/software vendors)
- Makes open-source version of UNICORE software available
- See http://www.unicore.org

Availability and Outlook

- Current version: UNICORE 4.0
  - open source release of full sources
  - available from UNICORE Forum web pages (www.unicore.org)
  - Upcoming project results to be made available likewise …
- Active participation in the GGF
  - workflow model
  - Grid operation (PKI issues, …)
- Moving towards supporting OGSA
  - UNICORE demonstrator by David Snelling …
- Interest in participating in new Grid projects
  - deployment and extensions
  - integration into OGSA framework
- Productization of UNICORE components
  - supported version available Q1/2003 from Pallas
  - include EUROGRID components

Further Information

- Contact grid@pallas.com
- WWW pages
  http://www.fz-juelich.de/unicore UNICORE Plus project
  http://www.unicore.org UNICORE Forum
  http://www.eurogrid.org EUROGRID project
  http://www.grid-interoperability.org GRIP project
- UNICORE test GRID
  http://www.fz-juelich.de/unicore-test FZ Jülich Test Grid
- Source code release
  http://www.unicore.org/downloads.htm UNICORE Forum

UNICORE and OGSA

- First step (demonstrated by David Snelling)
  - wrap the Client⇔Gateway protocol as Web Services
  - use the UNICORE servers in an OGSA-like way
  - simple "command-line" interface
  - continue to use the UNICORE workflow model and data formats
- Next step (concepts being developed)
  - remodel the UNICORE protocols as Grid Services
  - enable the Client to speak Grid Services
  - problem: no standard set of Grid Services defined yet …

Further directions OGSA

- translate from UNICORE workflow model to BPEL4WS
- "unbundle" UNICORE server functions, provide set of small-granular Grid Services
- use Grid Services to hook up to executions systems (replacing the current TSI)
- Vision
  - new-style Client speaks Grid Services and interacts with (many) Grid systems
  - new-style Servers use Grid Services to control execution systems, provide Grid Services to (many) Clients and applications

Pallas Company Profile

- Founded in 1991
- Since 2000 member of the ExperTeam group
- Staff: 60 (group 250)
- Business areas:
  - Pallas Performance
  - Pallas Security
  - Pallas Intelligence
- Location: Brühl, Dortmund
- Products, Consulting, Solutions, Services