A European GRID Approach - UNICORE, EUROGRID and GRIP

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Outline

- UNICORE history and motivation
- UNICORE approach
- UNICORE architecture and implementation
- UNICORE projects
- Availability and outlook

History and Motivation

- Once upon a time ...
  - there were many different HPC platforms
  - many organizations would run a "zoo" of systems

- Users of academic and industrial HPC centers had to cope with
  - primitive access mechanisms (telnet, ssh)
  - cumbersome authentication mechanisms (SecurID, S/key, …)
  - complicated batch systems (NQS, LL, …)
  - need to become experts of the systems they’re working on

- As a result
  - users stick to “their” systems
  - new platforms spell trouble
  - loss of flexibility at the centers

UNICORE Approach

- Provide a uniform work environment for users
  - access mechanism (browser, dedicated client, …)
  - authentication mechanisms (certificates, …)
  - hide system details (commands, data archives, batch systems, …)
  - define user-level resource and job model (task graph, …)
  - allow job monitoring and steering

- Lots of projects worldwide
  - SDSC Hotpage
  - AHPCRC TeraWeb
  - Mississippi State DMEFS
  - EnginFrame from NICE
  - …

- The UNICORE effort
  - originated from the leading German HPC centers in 1997
  - focused on seamless access within and across centers
  - emphasized security issues
  - avoided issues of resource pooling and brokering
  - decided to use the latest technology (Web-based client, Java)

- Achievements
  - demonstration of the architecture in 1999
  - working implementation in 2000/2001
  - production-ready implementations in 2001/2002

- Beneficial developments
  - broader scope (e.g. resource discovery and brokering)
  - emphasis on user interfaces for applications
  - open interfaces, protocols and (now) source
UNICORE Approach

- System architecture
  - multiple entry points, one per resource
  - cooperation between resources
  - allow for distributed computing

- Security mechanisms
  - user authentication by X.509 certificates
  - authorization handled per site
  - data integrity and confidentiality by reliance on SSL/https

- Implementation technique
  - emphasize portability, rely on standards
  - use Java for client and server components
  - build protocols on top of SSL/https
  - some (limited) use of XML

UNICORE Resource Model

- Usite
- Vsite
- Resources per Vsite
  - capacity
  - capability
- Resources are advertised to the client
  - pseudo-dynamic mode
- User submits jobs to Vsites
- Soon: automatic resource identification

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

- UNICORE Clients
- UNICORE Job Supervisor
- Secure Intranet
- Command or Routine I/F
- Cray NCE
- IBM LE
- SUN NQS
- UNICORE Batch interface

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
  - each DAG is signed with the private key
  - the Vsite executing a sub-job can check the sign

- Required trust
  - the user protects his/her private key
  - the CA is not compromised
**UNICORE – Job Submission and Execution**

- UNICORE Client
  - User certificate
  - Gateway
  - UPL requests/replies over SSL
- NJS Server
  - User login id
  - Job script over TCP
- Batch interface
  - Multi_optimization $\Rightarrow$ -O4
  - execute under user login id

- User certificate
- Gateway
- UPL requests/replies over SSL or sockets
- NJ/S Server
- User login id
- Job script over TCP
- Batch interface
- Multi_optimization $\Rightarrow$ -O4
- execute under user login id

**UNICORE Technology**

- Client and server components implemented in Java–2
- Authentication using X.509 certificates
  - UNICORE Plus project uses own public key infrastructure (PKI)
  - software can work with any other PKI
- 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
- Modeling of computational jobs and resources as Java objects (AJO)

**UNICORE GUI – Authentication**

- Unlock keystore
- User certificate
- CA certificate

**UNICORE GUI – Main Screen**

- Main dialog area
- Job panel
- Action buttons
- Monitor panel

**UNICORE GUI – Job Construction**

- Task graph
- Available sites
- Available machines

**UNICORE GUI – Task Definition**

- Files to be imported
- Files to be exported
- Job structure
- Script text
- Specify resources
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

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UNICORE Plus Project

- German national R&D project
- First production version (3.0) available since end of 2000
- Current phase: deployment and end-user evaluation
- Involvement of major German HPC centers
  - FZ Jülich
  - LRZ München
  - ZIB Berlin
  - P6 Paderborn
- Involvement of vendors
  - Cray/SGI
  - Hitachi
  - IBM
  - Siemens
- Involvement of ISVs
  - Pallas

EUROGRID – UNICORE in Europe

- Started as IST project end of 2000
- Based on UNICORE software release 3.0
- Domain-specific extensions
  - biology, meteorology, CAE
- General-purpose extensions
  - data transfer, resource brokering, ASP, interactive use
- Current phase: deployment, requirements analysis
- Involvement of European HPC centers
  - FZ Jülich
  - CNRS-IDRIS
  - DWD
  - University of Manchester
  - ICM Warsaw
- Involvement of industry
  - EADS CCR
  - debis Systemhaus
  - FECIT

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)

Bio–GRID

- PSE for bio–molecular applications
- Operate a GRID for bio–molecular simulations
- Develop interfaces to existing biological and chemical codes

Meteo–GRID

- Develop a relocatable version of DWD’s local weather prediction model
- ASP solution for on demand localized weather prediction

Meteo–Grid

- Ubiquitous access to local weather prediction software, developed at DWD and CSCS

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

- Coupled simulations of aircrafts (e.g., structure and electromagnetism)
- Goal: internal HPC portal for EADS engineers

EUROGRID Technology

- Provide HPC portal to engineers at Daimler-Chrysler and partners
- Develop GRID technology for computing cost estimates and billing

HPC–GRID

- Demonstrate a European HPC GRID testbed
- Develop new GRID applications
- Enable sharing of competence and know-how
- Agree on security standards, certification, access policies, ...

- CRAY T3E 900 (32 PE)
- NEC SX5/240
- Linux Cluster (8 PE)
- FZJ
- Intel Linux Cluster (32 PE)
- CRAY T3E - 400 (12 PE)
- CRAY T3E - 1200 (212 PE)
- Commit
- NEC SX5 cluster (60 PE)
- IBM Power4/200 PE, 1.3 TLOPS
- COMPAQ Linux Cluster (24 PE)

GRIP – Compatibility to Globus

- Started as IST project beginning of 2002
- To produce interoperability software for
  - using Globus resources from UNICORE
  - submitting UNICORE jobs from Globus
- To enhance the EUROGRID resource broker to span UNICORE and Globus
- To evaluate the interoperability with
  - biomolecular applications from ICM
  - on-demand weather prediction from DWD
- Current phase: requirements analysis, architecture specification
- Argonne National Labs is participating!

GRIP Partners

- HPC Centers
  - FZ Jülich (D)
  - ICM Warsaw (PL)
  - Univ. Manchester (UK)
  - Univ. Southampton
- Users
  - Deutscher Wetterdienst
- Integration
  - Pallas (Project Coordinator)
  - Argonne National Labs

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

- Current version: UNICORE 3.6
  - missing functionality: control tasks (If, Repeat, …)
  - available for project partners and on request
  - starting May 2002: access to full sources

- Upcoming production version: UNICORE 4.0
  - supports control tasks
  - many improvements to the user interface
  - release in July/August timeframe
  - partners and source repository will be updated

- Results from EUROGRID and GRIP to be made available in a similar manner …

Open Issues

- Running a PKI in the real world
  - provide reasonable level of security
  - don’t offend users …

- Cope with security people
  - source IP-filtering makes access from anywhere impossible …
  - work with stricter rules for outgoing IP

- Obnoxious authentication systems
  - SecurID and skey will require pass codes for trivial operations …

- Get more user input
  - users of classic HPC centers
  - industrial users (ASP-like model)

Further Information

- Leaflets (on a desk in the lobby)

- WWW pages
  - http://www.fz-juelich.de/unicore
  - http://www.unicore.org
  - http://www.eurogrid.org
  - http://www.grid-interoperability.org

  UNICORE Plus project
  UNICORE Forum
  EUROGRID project
  GRIP project