European Middleware Initiative

UNICORE 6

# Role, Objectives and Migration Plans to the European Middleware Initiative (EMI)

http://www.unicore.eu

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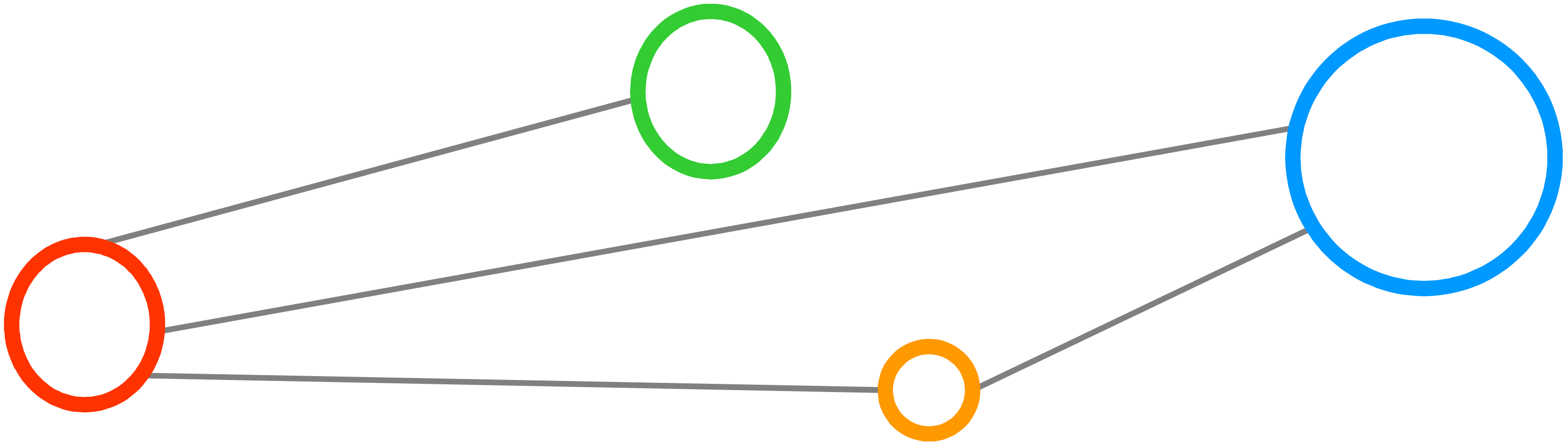
JÜLICH
FORSCHUNGSZENTRUM

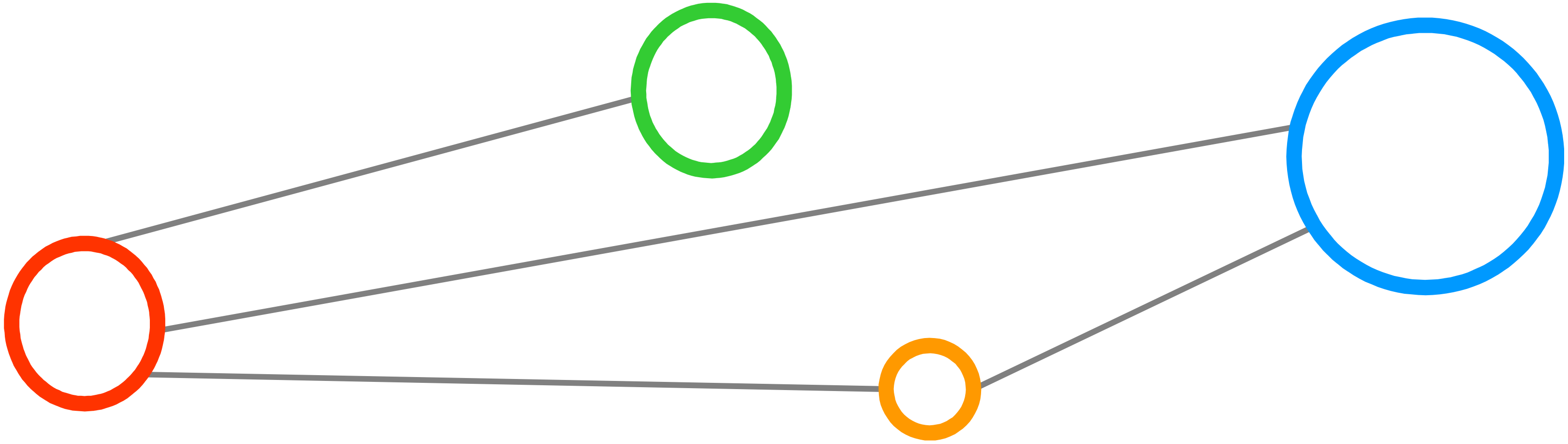
# Outline



# Outline

- UNICORE 101 & Usage Examples
- Role as HPC-driven Grid Middleware
  - Traditional role and emerging role in HTC
- Objectives and Migration Plans
  - Migration to Common Client API
  - Migration to Common EMI Security Infrastructure
  - Common Registry Service Objective
  - PGI-compliance for Compute and Data Objective
  - Common Attribute-based Authorization
  - ***Moving towards potential EMI Architecture***
  - Other Potential Objectives
- Summary

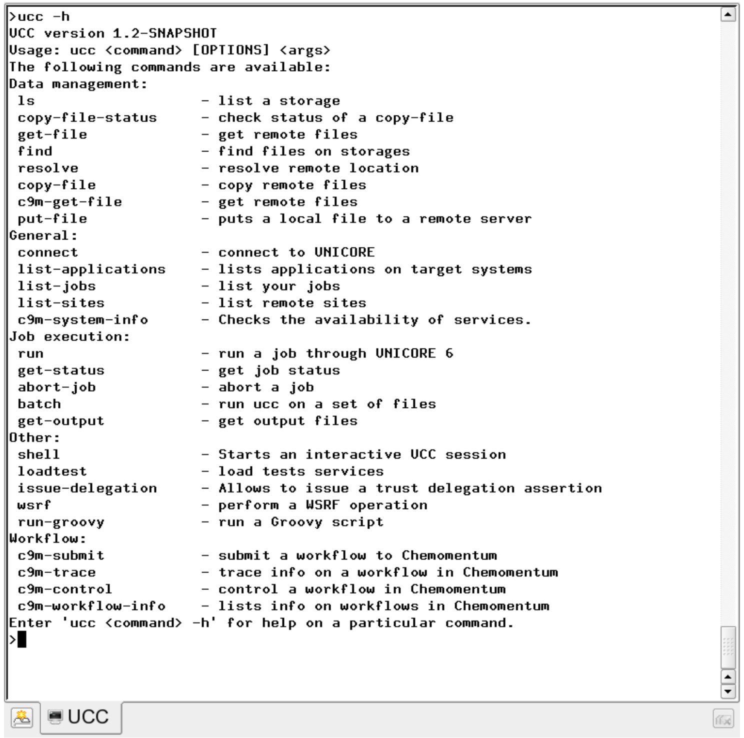
# UNICORE 101



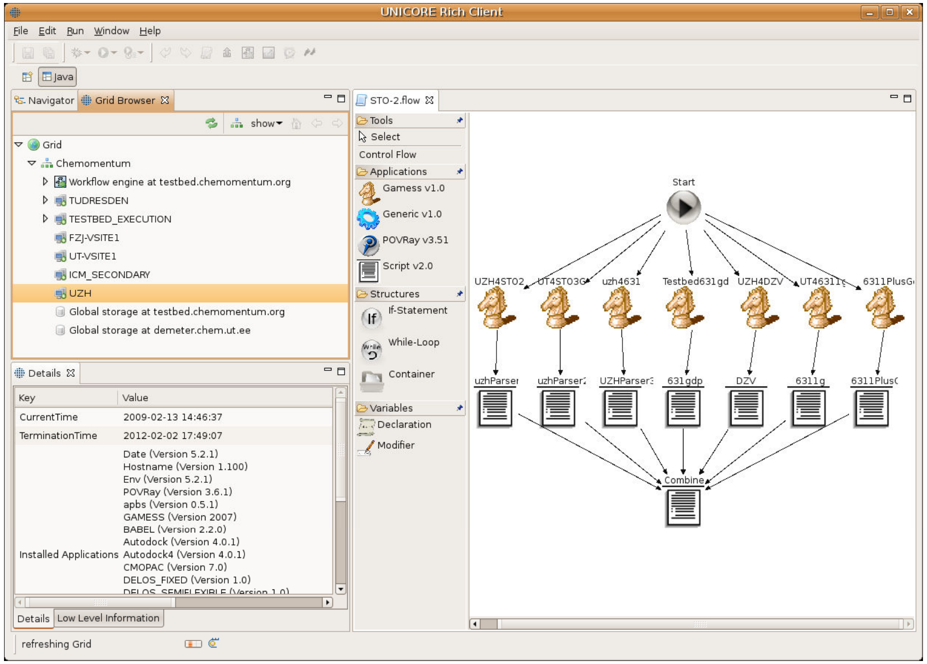
# Guiding Principles, Implementation Strategies

- **Open source** under BSD license with software hosted on SourceForge
- **Standards-based**: OGSA-conform, WS-RF 1.2 compliant
- Open, extensible **Service-Oriented Architecture** (SOA)
- **Interoperable** with other Grid technologies
- Seamless, secure and intuitive following a vertical end-to-end approach
- Mature **Security**: X.509, proxy and VO support
- **Workflow** support tightly integrated while being extensible for different workflow languages and engines for domain-specific usage
- **Application integration** mechanisms on the client, services and resource level
- Variety of **clients**: graphical, command-line, API, portal, etc.
- Quick and **simple installation** and configuration
- Support for many operating systems (Windows, MacOS, Linux, UNIX) and batch systems (LoadLeveler, Torque, SLURM, LSF, OpenCCS)
- Implemented in **Java** to achieve platform-independence

# Clients & APIs



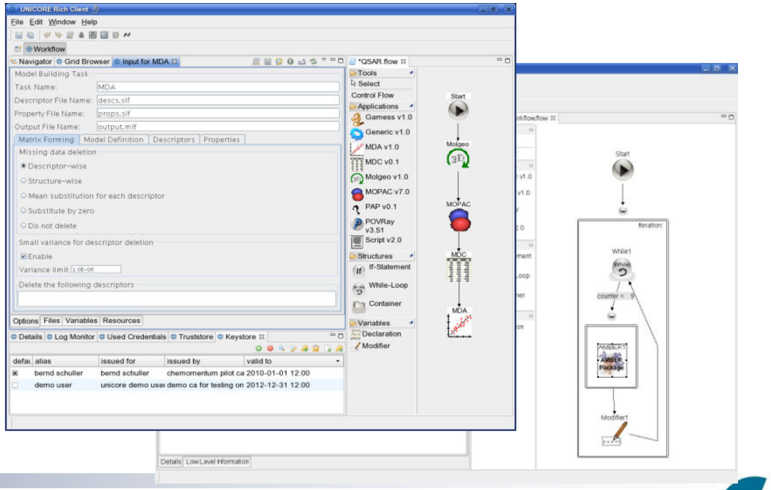
```
>ucc -h
UCC version 1.2-SNAPSHOT
Usage: ucc <command> [OPTIONS] <args>
The following commands are available:
Data management:
 ls                     - list a storage
 copy-file-status       - check status of a copy-file
 get-file               - get remote files
 find                   - find files on storages
 resolve                - resolve remote location
 copy-file              - copy remote files
 c9m-get-file           - get remote files
 put-file               - puts a local file to a remote server
General:
 connect                - connect to UNICORE
 list-applications      - lists applications on target systems
 list-jobs              - list your jobs
 list-sites             - list remote sites
 c9m-system-info        - Checks the availability of services.
Job execution:
 run                    - run a job through UNICORE 6
 get-status             - get job status
 abort-job              - abort a job
 batch                  - run ucc on a set of files
 get-output             - get output files
Other:
 shell                  - Starts an interactive UCC session
 loadtest               - load tests services
 issue-delegation       - Allows to issue a trust delegation assertion
 wsrf                   - perform a WSRF operation
 run-groovy             - run a Groovy script
Workflow:
 c9m-submit             - submit a workflow to Chemomentum
 c9m-trace              - trace info on a workflow in Chemomentum
 c9m-control            - control a workflow in Chemomentum
 c9m-workflow-info      - lists info on workflows in Chemomentum
Enter 'ucc <command> -h' for help on a particular command.
>
```



Grid
- Chemomentum
  - Workflow engine at testbed.chemomentum.org
  - TUDRESDEN
  - TESTBED_EXECUTION
  - FZJ-VSITE1
  - UT-VSITE1
  - ICM_SECONDARY
  - UZH
  - Global storage at testbed.chemomentum.org
  - Global storage at demeter.chem.ut.ee

Details

| Key | Value |
|---|---|
| CurrentTime | 2009-02-13 14:46:37 |
| TerminationTime | 2012-02-02 17:49:07 |
| Installed Applications | Date (Version 5.2.1)<br>Hostname (Version 1.100)<br>Env (Version 5.2.1)<br>POVRay (Version 3.6.1)<br>apbs (Version 0.5.1)<br>GAMESS (Version 2007)<br>BABEL (Version 2.2.0)<br>Autodock (Version 4.0.1)<br>Autodock4 (Version 4.0.1)<br>CMOPAC (Version 7.0)<br>DELOS_FIXED (Version 1.0)<br>DELOS_SEMIFLEXIBLE (Version 1.0) |



Model Building Task

Task Name: MDA

Descriptor File Name: descs.slf

Property File Name: props.slf

Output File Name: output.mlf

Matrix Forming | Model Definition | Descriptors | Properties

Missing data deletion

- ● Descriptor-wise
- ○ Structure-wise
- ○ Mean substitution for each descriptor
- ○ Substitute by zero
- ○ Do not delete

Small variance for descriptor deletion

☒ Enable

Variance limit 1.0E-06

Delete the following descriptors

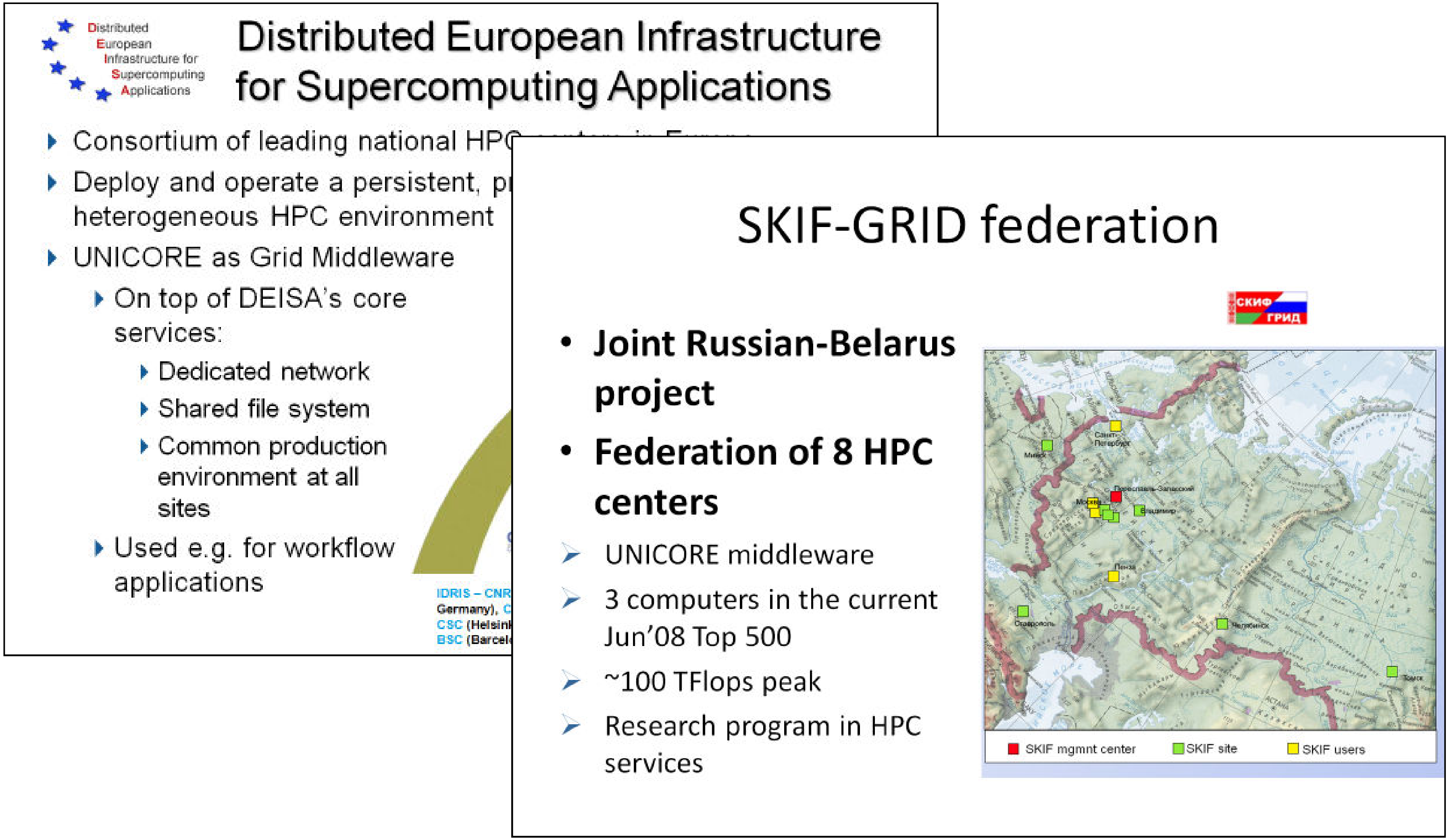
Options | Files | Variables | Resources

Details | Log Monitor | Used Credentials | Truststore | Keystore

| defau | alias | issued for | issued by | valid to |
|---|---|---|---|---|
| ☒ | bernd schuller | bernd schuller | chemomentum pilot ca | 2010-01-01 12:00 |
| □ | demo user | unicore demo use | demo ca for testing on | 2012-12-31 12:00 |

HiLA

# Usage in Supercomputing



Distributed European Infrastructure for Supercomputing Applications

## Distributed European Infrastructure for Supercomputing Applications

- Consortium of leading national HPC centers in Europe
- Deploy and operate a persistent, pr
  heterogeneous HPC environment
- UNICORE as Grid Middleware
  - On top of DEISA's core services:
    - Dedicated network
    - Shared file system
    - Common production environment at all sites
  - Used e.g. for workflow applications

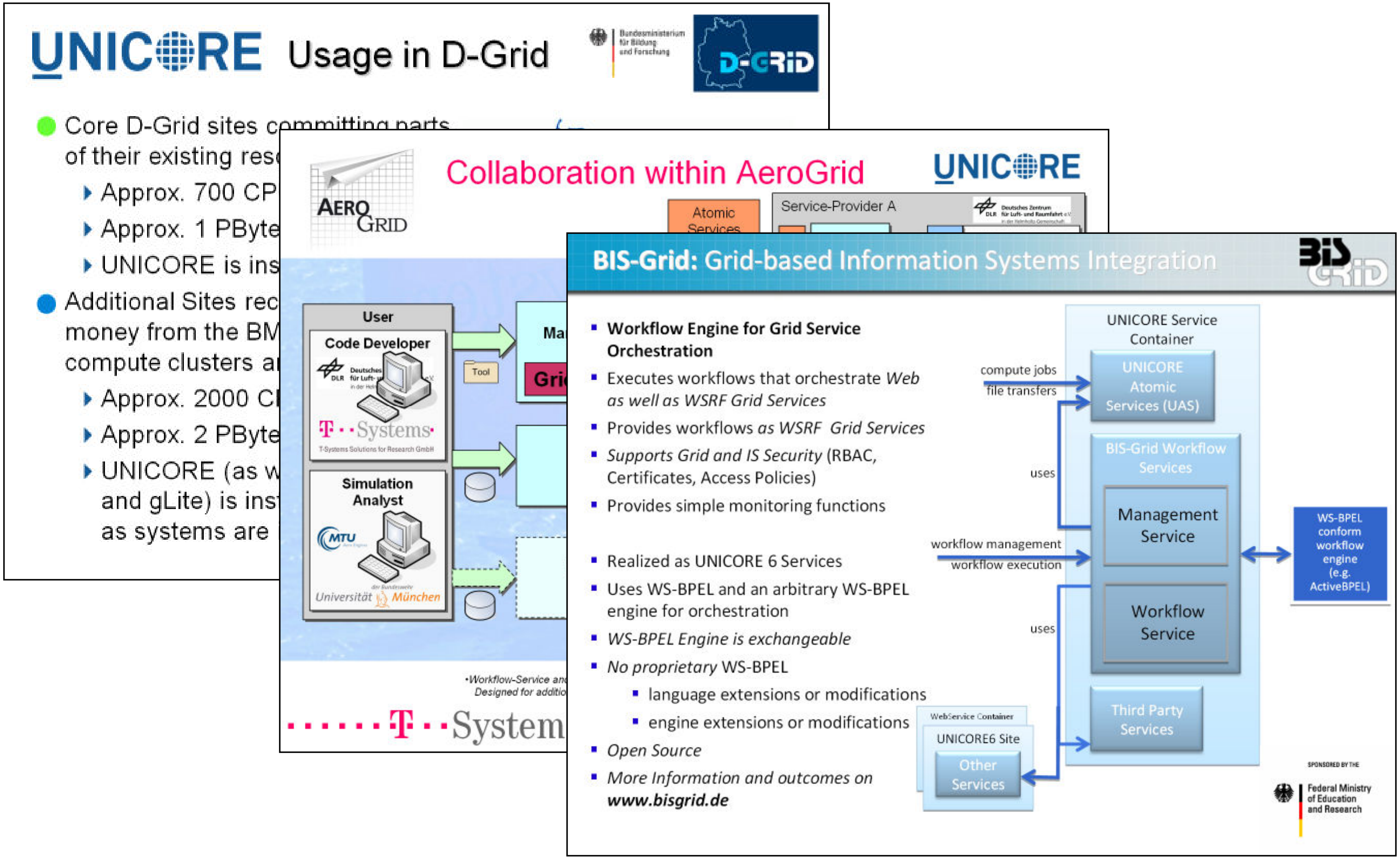
IDRIS – CNR
Germany), C
CSC (Helsink
BSC (Barcel

## SKIF-GRID federation

- **Joint Russian-Belarus project**
- **Federation of 8 HPC centers**
  - UNICORE middleware
  - 3 computers in the current Jun'08 Top 500
  - ~100 TFlops peak
  - Research program in HPC services

Slide courtesy of Alexander Moskovsky (Moscow State University)

# Usage in National Grids



## UNICORE Usage in D-Grid

Bundesministerium für Bildung und Forschung
D-GRID

- Core D-Grid sites committing parts of their existing res
  - Approx. 700 CP
  - Approx. 1 PByte
  - UNICORE is ins
- Additional Sites rec money from the BM compute clusters a
  - Approx. 2000 C
  - Approx. 2 PByte
  - UNICORE (as w and gLite) is ins as systems are

## Collaboration within AeroGrid

AERO GRID
UNICORE
Atomic Services
Service-Provider A
Deutsches Zentrum für Luft- und Raumfahrt e.V. in der Helmholtz-Gemeinschaft
User
Code Developer
T··Systems·
T-Systems Solutions for Research GmbH
Simulation Analyst
MTU
Universität der Bundeswehr München
Tool
Ma
Gri

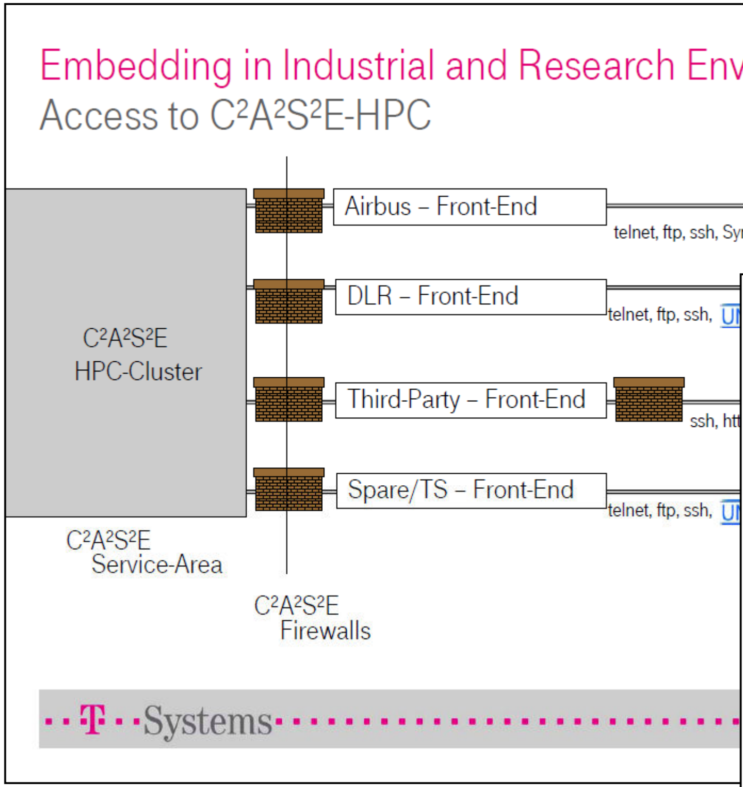
•Workflow-Service an Designed for additio

## BIS-Grid: Grid-based Information Systems Integration

- **Workflow Engine for Grid Service Orchestration**
- Executes workflows that orchestrate *Web as well as WSRF Grid Services*
- Provides workflows *as WSRF Grid Services*
- *Supports Grid and IS Security* (RBAC, Certificates, Access Policies)
- Provides simple monitoring functions
- Realized as UNICORE 6 Services
- Uses WS-BPEL and an arbitrary WS-BPEL engine for orchestration
- *WS-BPEL Engine is exchangeable*
- *No proprietary* WS-BPEL
  - language extensions or modifications
  - engine extensions or modifications
- *Open Source*
- *More Information and outcomes on* ***www.bisgrid.de***

Slide courtesy of André Höing (TU Berlin)

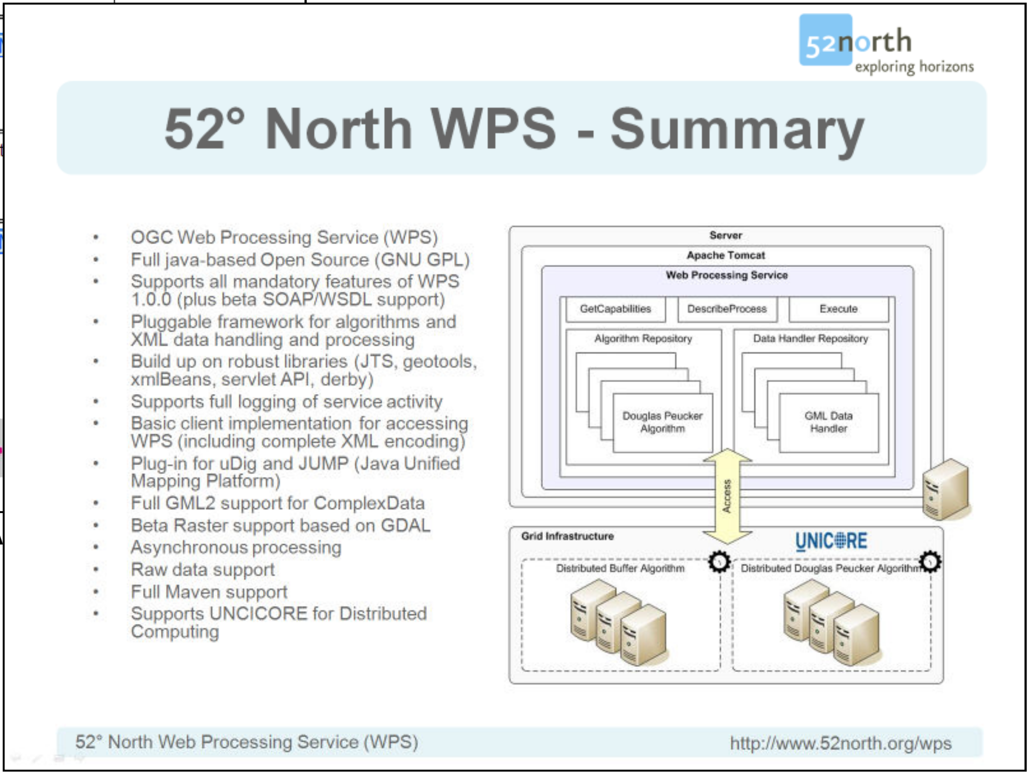
# Usage in Commercial Areas



## Embedding in Industrial and Research Environments:

Access to C²A²S²E-HPC

Slide courtesy of A



52north exploring horizons

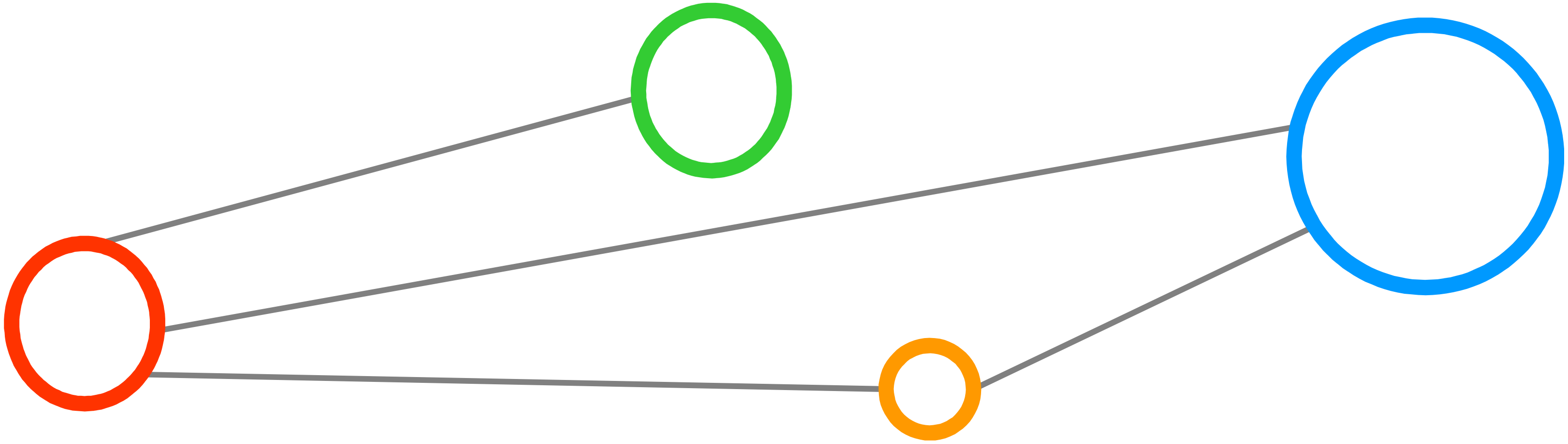
## 52° North WPS - Summary

- OGC Web Processing Service (WPS)
- Full java-based Open Source (GNU GPL)
- Supports all mandatory features of WPS 1.0.0 (plus beta SOAP/WSDL support)
- Pluggable framework for algorithms and XML data handling and processing
- Build up on robust libraries (JTS, geotools, xmlBeans, servlet API, derby)
- Supports full logging of service activity
- Basic client implementation for accessing WPS (including complete XML encoding)
- Plug-in for uDig and JUMP (Java Unified Mapping Platform)
- Full GML2 support for ComplexData
- Beta Raster support based on GDAL
- Asynchronous processing
- Raw data support
- Full Maven support
- Supports UNCICORE for Distributed Computing

52° North Web Processing Service (WPS) http://www.52north.org/wps

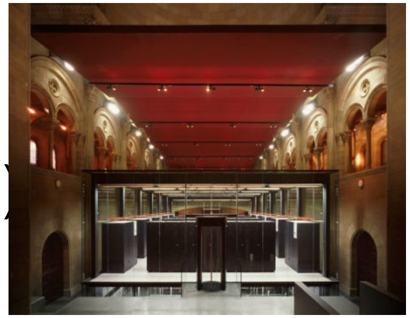
Slide courtesy of Bastian Baranski (52° North & University Münster)

# Role as HPC-Driven Grid Middleware



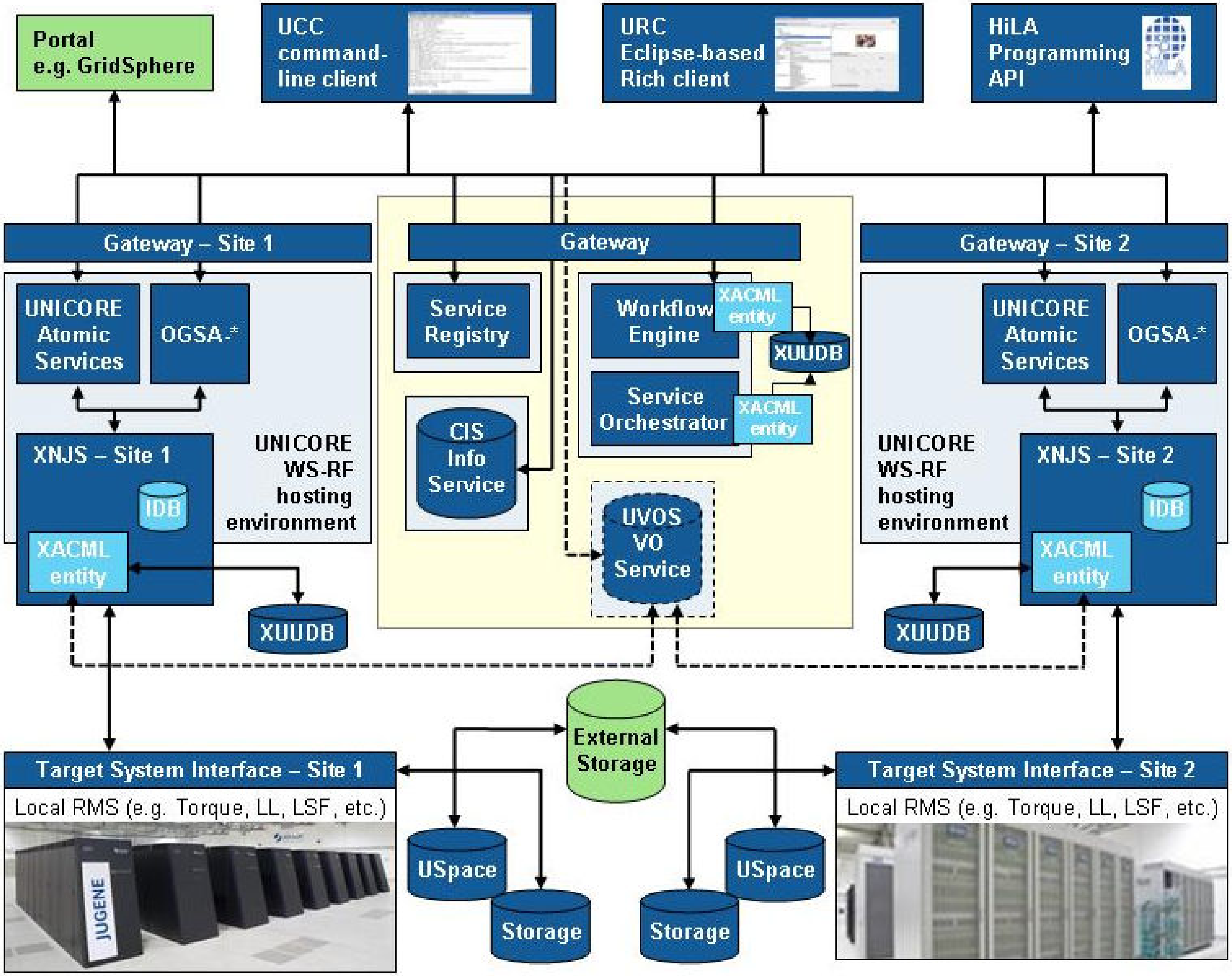
# Grid driving High Performance Computing (HPC)

- Used in
  - DEISA (European Distributed Supercomputing Infrastructure)
  - National German Supercomputing Center NIC
  - Gauss Center for Supercomputing
    (Alliance of the three German HPC centers & official National Grid Initiative for Germany in the context of EGI)
  - PRACE (European PetaFlop HPC Infrastructure) – starting-up
- Traditionally taking up major requirements from i.e.
  - HPC users (i.e. MPI, OpenMP)
  - HPC user support teams
  - HPC operations teams
  - …and via SourceForge Platform



sourceforge FIND AND DEVELOP OPEN SOURCE SOFTWARE

# UNICORE Architecture Overview



scientific clients and applications

authentication

emerging standard interfaces

Grid services hosting

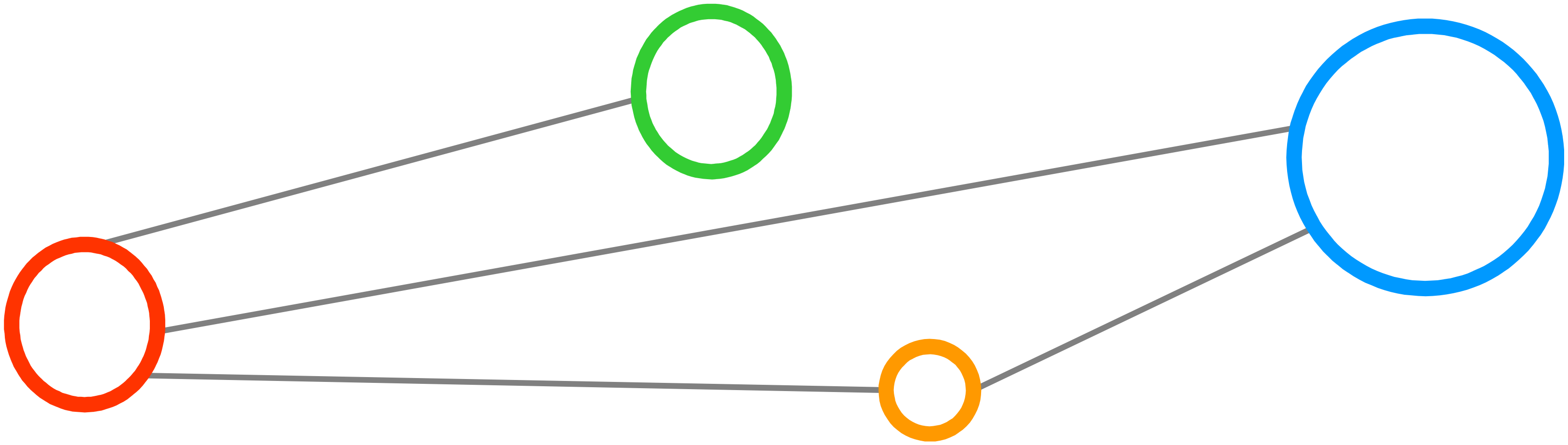
job incarnation & authorisation

parallel scientific jobs of multiple end-users on target systems

# EMI and High Throughput Computing (HTC)

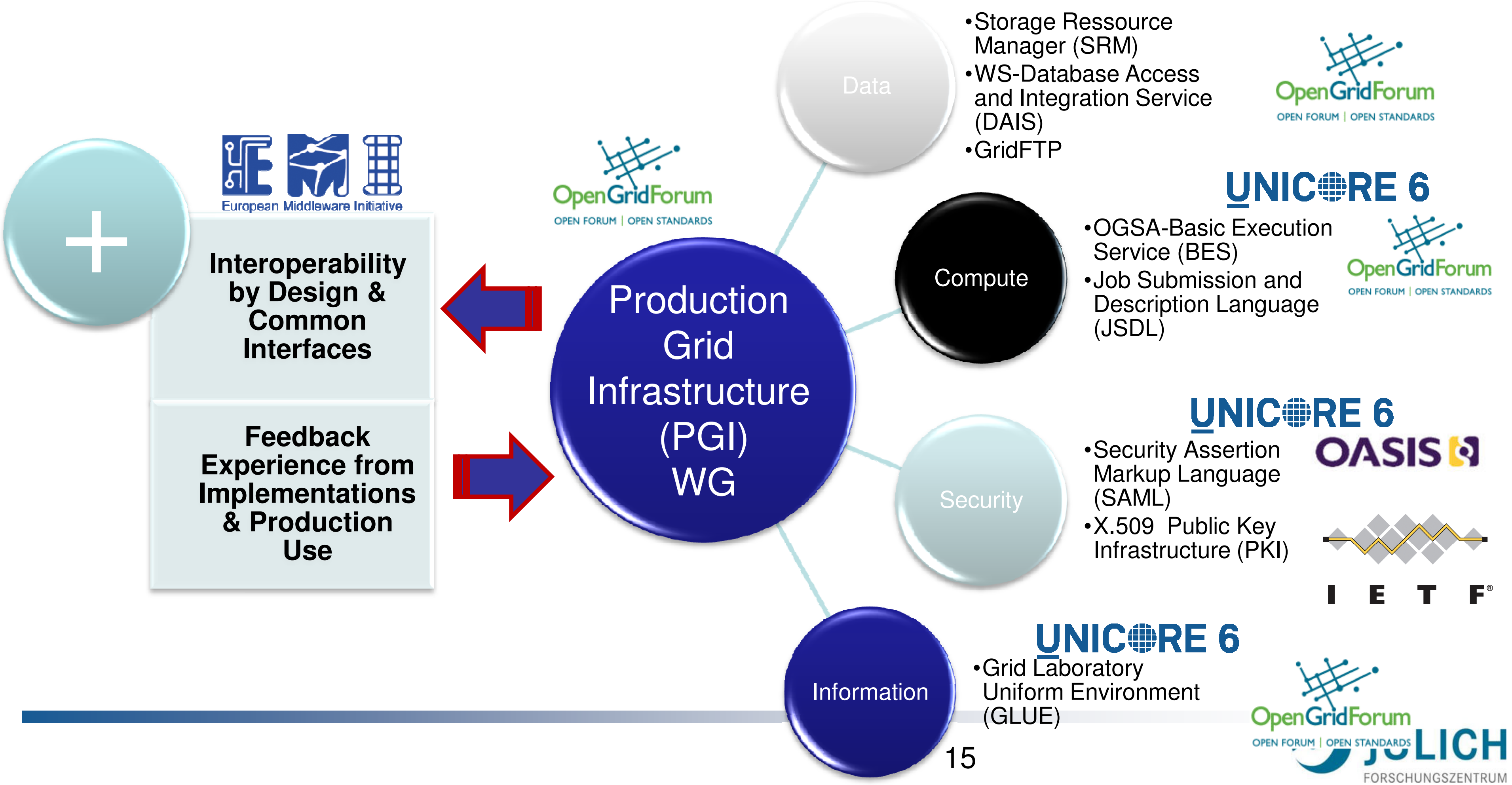
- UNICORE can be used in non HPC-focussed environments
  - German National Grid D-Grid and some of there communities
  - High Throughput Computing (HTC) possible with UNICORE
  - EMI will be possibly deployed on many HTC-driven Grids
- Role towards the European Middleware Initiative (EMI)
  - Stronger support for distributed data and storage technologies
  - Aligning with the key features of other EMI middleware such as ARC & gLite (e.g. pool accounts)
  - Integrate requirements arising from HTC-driven environments

# Objectives and Migration Plans



# General Paradigm: Adopting Open Standards

- Adopt and drive efforts of the OGF PGI-WG



**Interoperability by Design & Common Interfaces**

**Feedback Experience from Implementations & Production Use**

Production Grid Infrastructure (PGI) WG

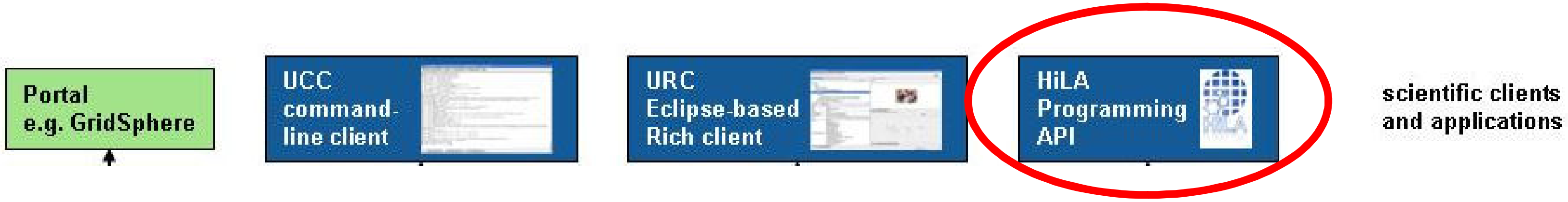
Data
- Storage Ressource Manager (SRM)
- WS-Database Access and Integration Service (DAIS)
- GridFTP

Compute
- OGSA-Basic Execution Service (BES)
- Job Submission and Description Language (JSDL)

Security
- Security Assertion Markup Language (SAML)
- X.509 Public Key Infrastructure (PKI)

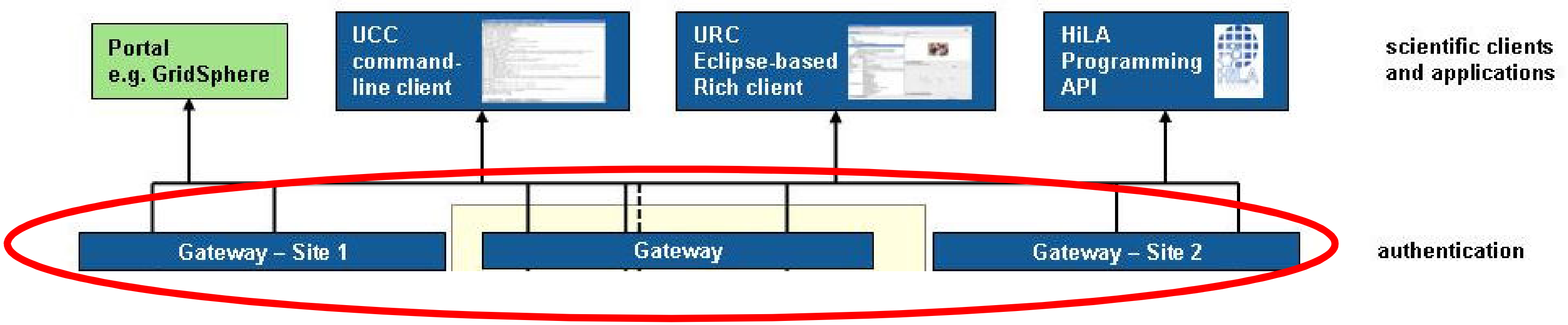
Information
- Grid Laboratory Uniform Environment (GLUE)

# Migration to Common Client API



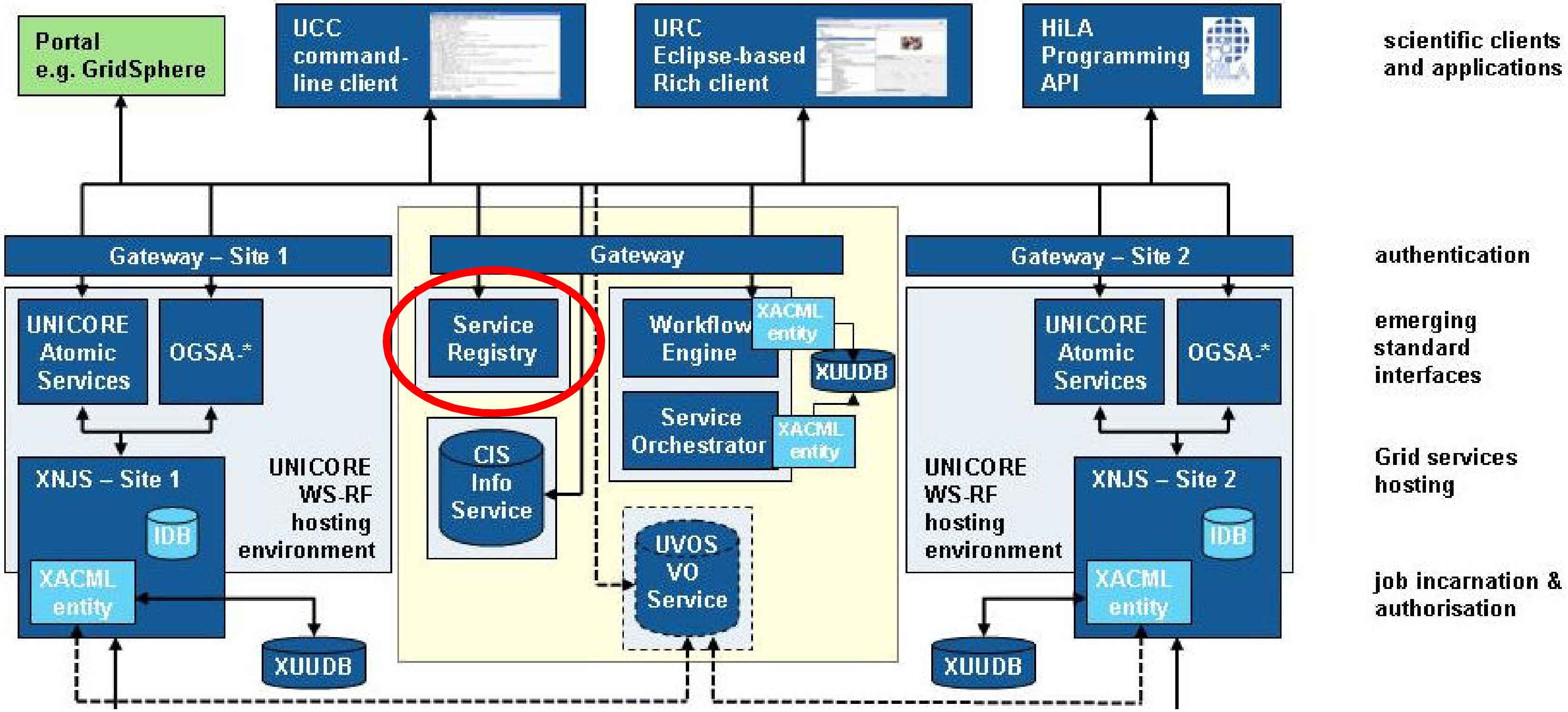
- Offer Higher Level Application Programming API (HILA) as potential common client API in EMI
  - Easy programming API with non UNICORE-based Grid abstractions (e.g. Grid, Site, etc.)
  - Potential integration of emerging standards of the OGF Production Grid Infrastructure (PGI) working group
  - Access to all PGI-compliant Grid middlewares and thus to ARC (e.g. A-Rex) and gLite (e.g. computing element) once PGI is adopted
- Potential access of PGI-compliant middleware (UNICORE, ARC, gLite, …) from other available clients as well

# Migration to Common EMI Security Infrastructure



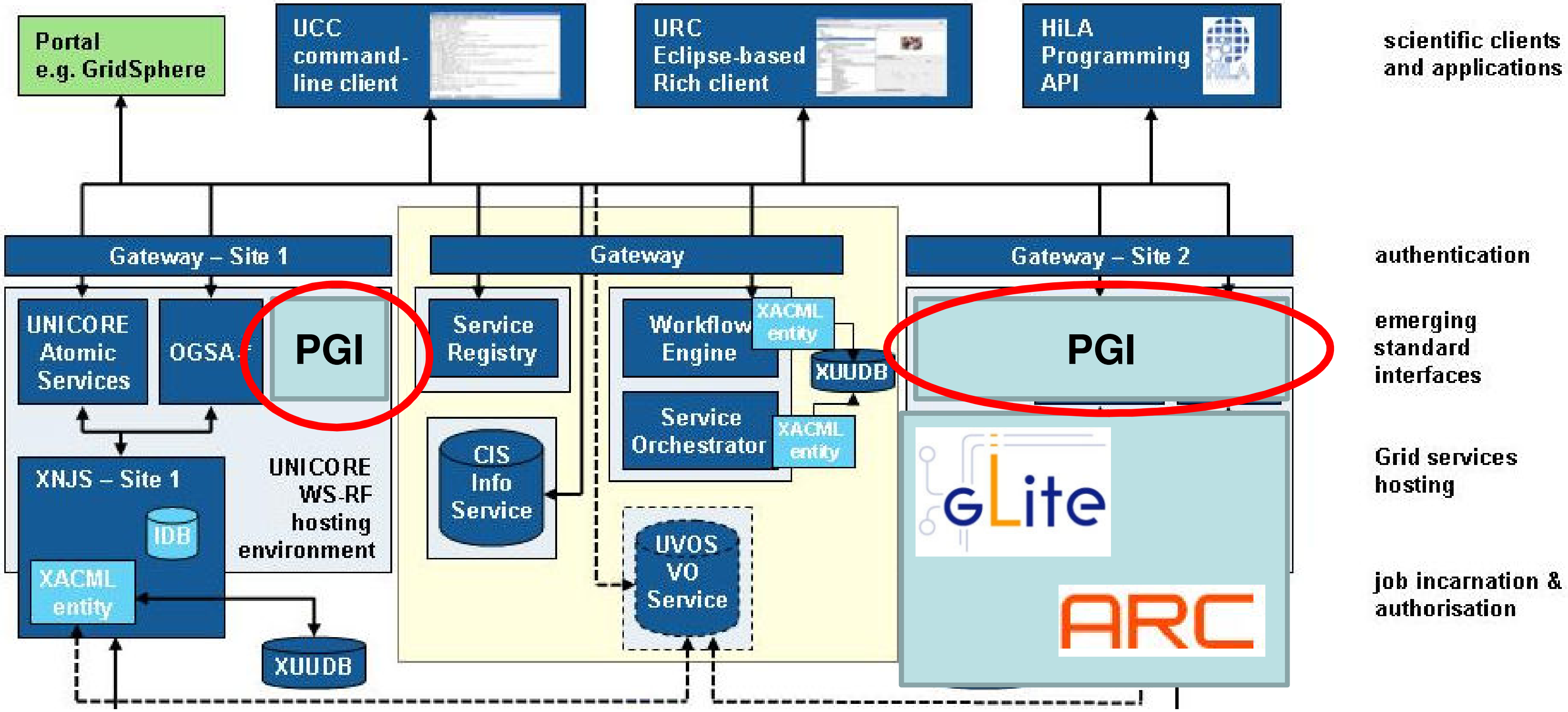
- Take up of common EMI security infrastructure
  - Aligned with efforts of the OGF PGI working group
  - Move away from Grid Security Infrastructure (GSI)
  - Enables a broader access from non-Grid environments (i.e. Web) & broader support for tooling to satisfy industry needs
- Offer Gateway as a common EMI authentication component
  - Potentially merging functionality with gLite trust manager, etc.
  - Exploring potentials for Shibboleth-based EMI federations

# Common Registry Service Objective



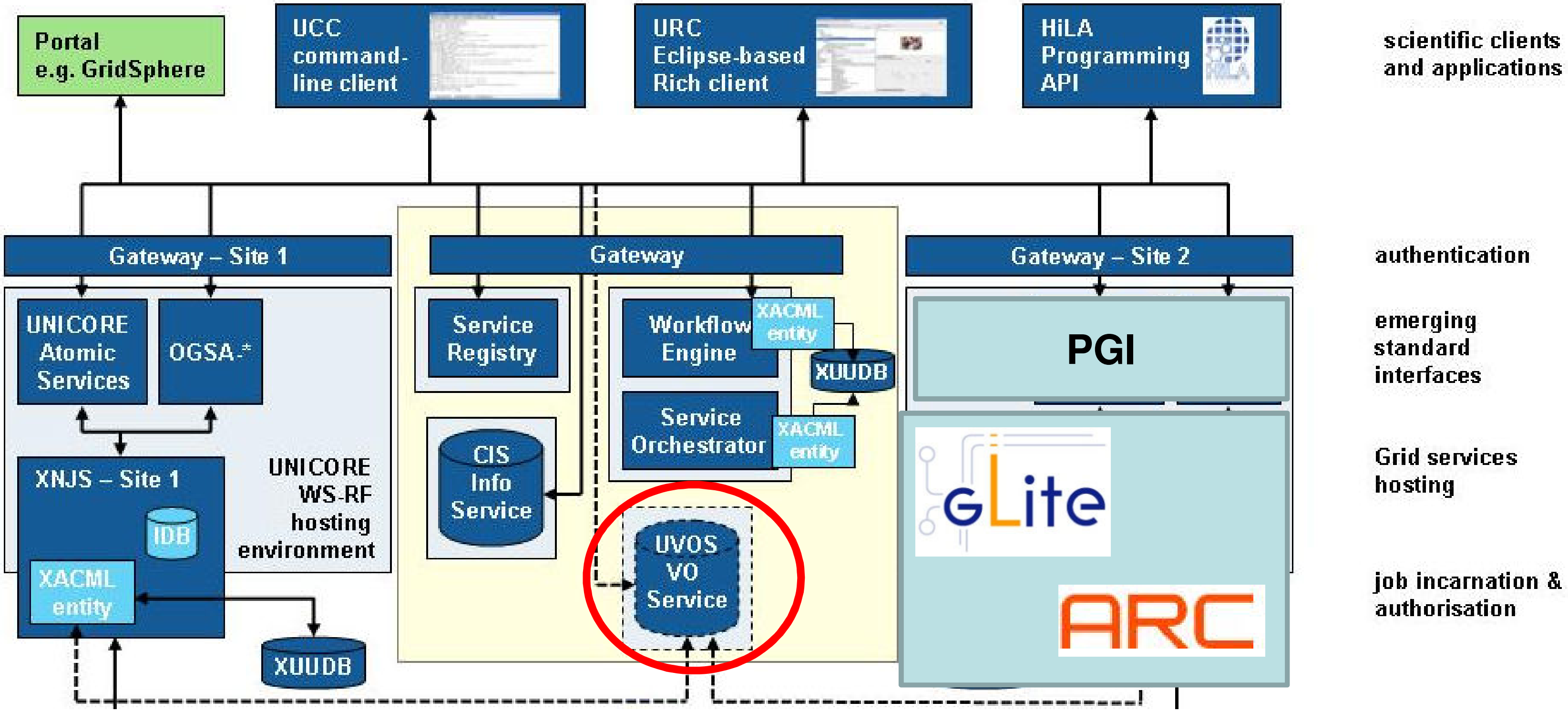
- Goal: common registry service for UNICORE, ARC & gLite
  - Outphasing of the WS-RF-based UNICORE Service Registry

# PGI-compliance for Compute & Data Objective



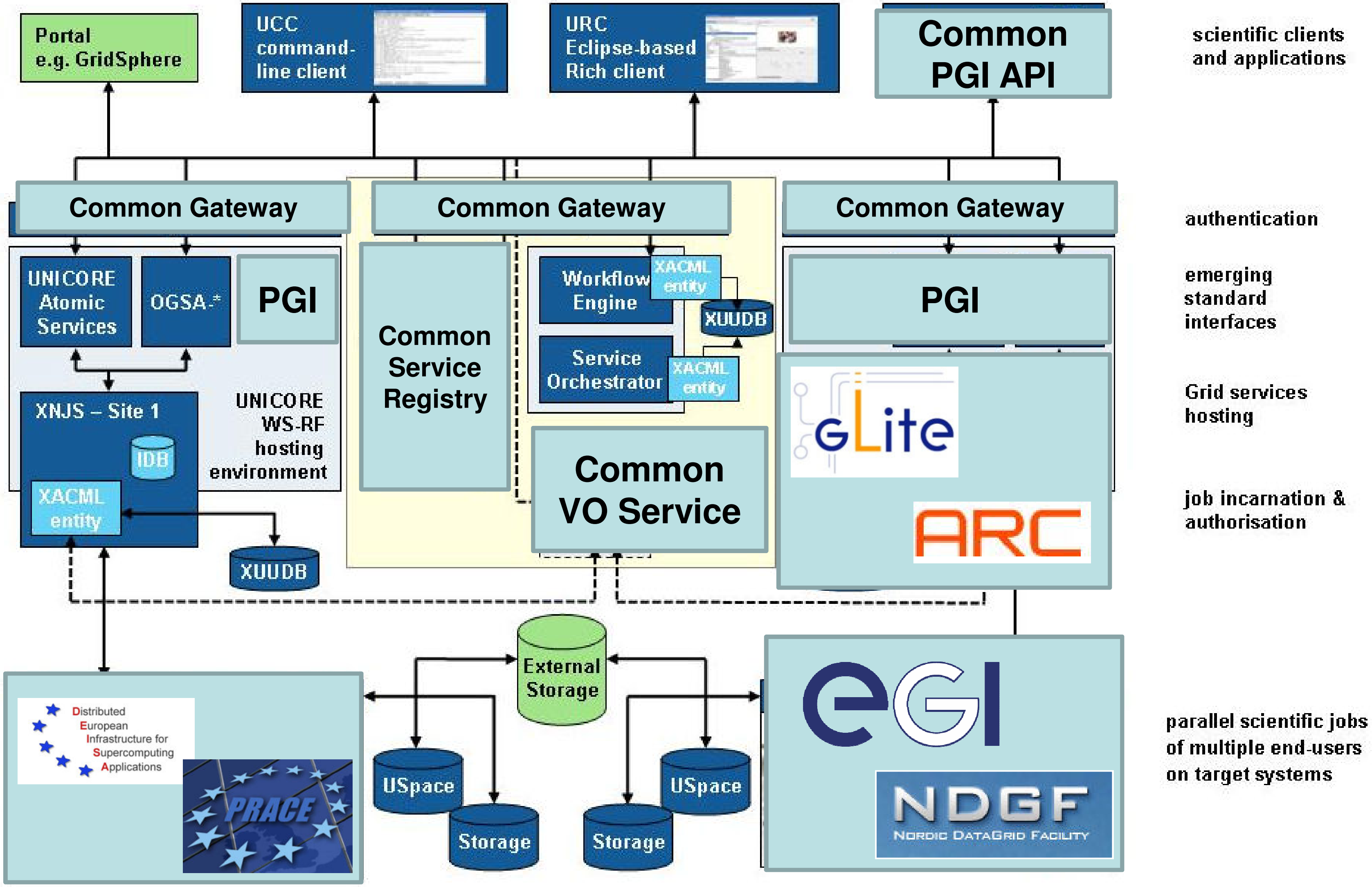
- Take up of emerging PGI standards driven by EMI for compute and data interfaces to access also gLite & ARC
  - Parallel Interfaces to proprietary UNICORE Atomic Services

# Common Attribute-based Authorization



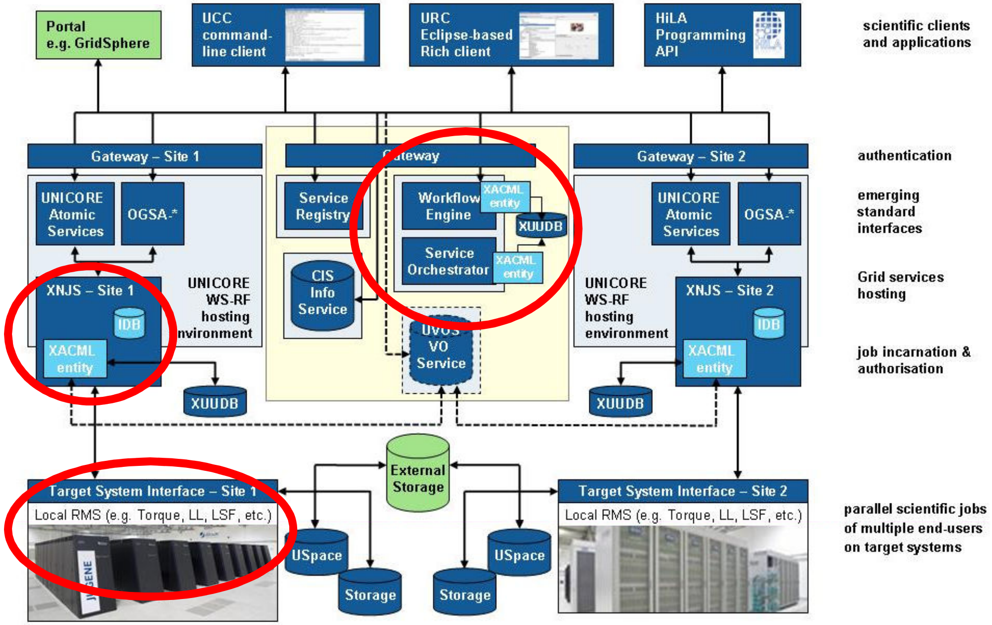
- Take up of a common EMI attribute-based authorization service support and open interfaces for Virtual Organizations
  - Push of Security Assertion Markup Language (SAML) usage

# Moving towards potential EMI Architecture



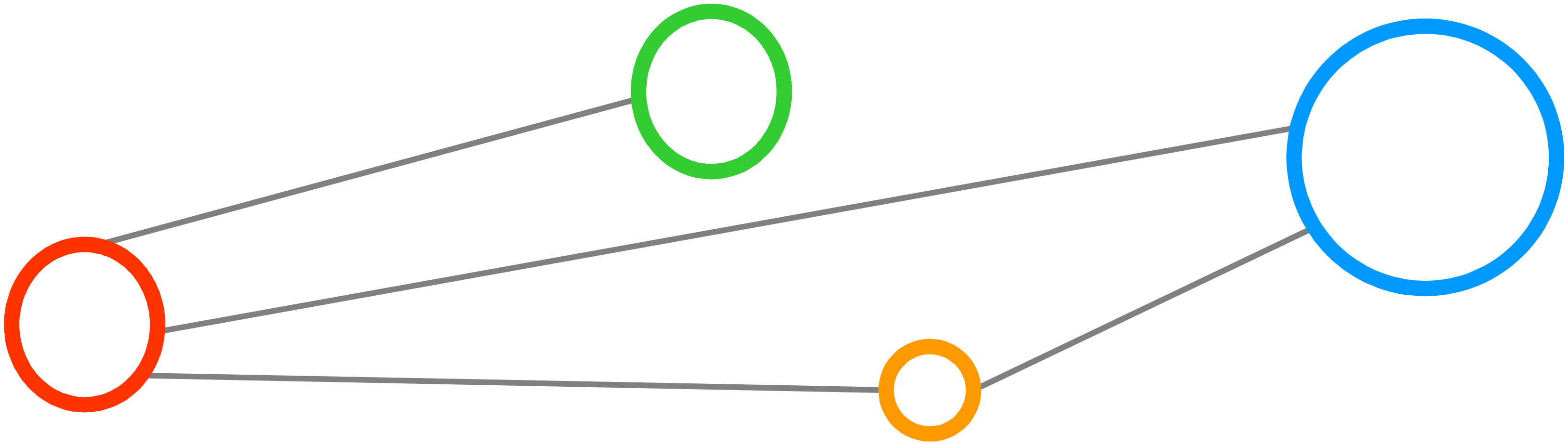
# Other Potential Objectives

- Workflow (maybe out of EMI scope, but important)
  - Workflow functionality make job chains possible across multiple sites
  - Workflow Engine & Service Orchestrator good base for EMI

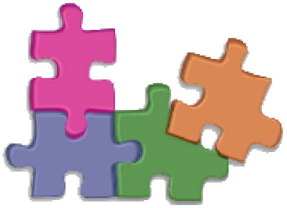


- Strong execution backend XNJS and TSI
  - Provide support for many operating and batch systems with continued development since ~10 years
  - Strong MPI support may (will) become highly relevant for EMI in the “economy of scales” → we reached peta-scale already…

# Summary



# Summary of Components of Interest for EMI



- All components are subject to be harmonized
- Security
  - UNICORE Gateway (i.e. authentication)
  - UNICORE VO Service (UVOS) (i.e. Attribute Authority)
  - XACML Entity (i.e. attribute-based authorization decisions)
- Compute
  - XNJS, UNICORE Atomic Services & OGSA-BES (i.e. execution)
  - Workflow Engine to be compliant with EMI execution interface
- Information
  - Service Registry (i.e. information about available Grid services)
- Data
  - UNICORE Atomic Services (i.e. data)

# General Summary

- UNICORE is a ready-to-run European Grid Technology including client and server software highly relevant for EMI
- Provides a seamless, secure, and intuitive access to different distributed computing and data resources
- All components are available as open source under BSD License on SourceForge & support for science and industry
- Traditional role as HPC-driven middleware and more recently also usable in Grid environments (i.e. High Throughput Computing)
- Commitment to open standards to support a common set of interfaces and protocols of emerging components of the EMI

# UNICORE

**software, source code, documentation, tutorials, mailing lists, community links, and more:**

## http://www.unicore.eu