






Fact-Sheet EU-IndiaGrid Interoperability Scenario


Context

- A real-world use case demonstrating how OMII-Europe components can be used in e-Infrastructures
- A particular set of OMII-Europe components mapped to interoperability requirements of one project

Background: e-Infrastructure Islands of Europe and India

- Distributed European Infrastructure for Supercomputing Applications (DEISA)
 - Supercomputing / High Performance Computing (HPC) application-driven infrastructure suitable for large-scale and massively parallel computing
 - Link: <http://www.deisa.org>
 - Deployed non WS-based UNICORE 5 that uses a proprietary job description language named as Abstract Job Object (AJO) and a proprietary protocol named as UNICORE Protocol Layer (UPL), mostly using security setups with full X.509 certificates
- Enabling Grids for e-Science (EGEE)
 - Mainly High Energy Physics (HEP) community and other communities providing shared resources for low-scale and medium-scale computing, but mostly no HPC
 - Link: <http://www.eu-egee.org>
 - Deployed non WS-based gLite/lcg that uses a proprietary job description language named as Job Description Language (JDL) and proprietary protocols for component interactions
- Indian National Grid (GARUDA)
 - Emerging Grid infrastructure that connect 17 cities within India with a very heterogeneous set of Grid resources that allow for low- to medium-scale computing and rare HPC
 - Link: <http://www.garudaindia.in/>
 - Deployed Globus Toolkit that uses proprietary job description languages named as Resource Specification Language (RSL) and proprietary protocols for job submits
- All three Grids are in 2007 not technically interoperable and had less adoption of standards in the past. Also, the security setup between these three Grids and its middleware was non-interoperable.

Requirements of EU-IndiaGrid Project

- EU-IndiaGrid builds a Grid-enabled e-Science Community,
Link: <http://www.euindiagrid.eu/>
 - It brings together over 500 multi-disciplinary organisations to build an e-Science community and thus develops a sustained base of potential users from key science domains across Europe and India
 - One particular use case is that EU-IndiaGrid e-Scientists work on quantum atomistic simulations that are very demanding in terms of CPU and memory requirements.
 - Among some other scientific packages, the programs VASP and WIEN2K are used
 - Both of them are already ported on all three Grid environments
 - Idea: Use the seamless access of the different Grid infrastructures GARUDA, EGEE and DEISA for different kinds of scalable calculations in terms of the order of simulated atoms
 - Serial versions of the package are suitable to run in GARUDA and EGEE. But those serial versions are limited to study very small systems (e.g. in the order of few tens of atoms).
 - Small parallel versions (e.g. using 2-8 CPUs in parallel) are suitable to run in EGEE or DEISA and allow for simulation of larger systems (e.g. less than hundred of atoms)
 - Large parallel versions to go beyond the previous mentioned sizes of systems for atomistic simulations are only suitable for DEISA HPC platforms (e.g. thousands of atoms)
 - **GOAL: More variety of resources for scientific applications requiring different levels of scaling within GARUDA, EGEE, and DEISA using OMII-Europe components**
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Description of interoperability scenario

- This interoperability scenario is a demonstrator of how EU-IndiaGrid e-Scientists can seamlessly use all three infrastructures GARUDA, EGEE and DEISA to improve their daily work
- This scenario represents a whole class of similar interoperability scenarios with similar requirements for interoperability between Globus-based, gLite-based and UNICORE-based Grid infrastructures
- It shows how OMII-Europe components are used to enable interoperability between upcoming standard-compliant versions of UNICORE 6, gLite, and Globus Toolkit 4 that all are deployed or planned to be deployed in the very different infrastructures GARUDA, EGEE and DEISA very soon

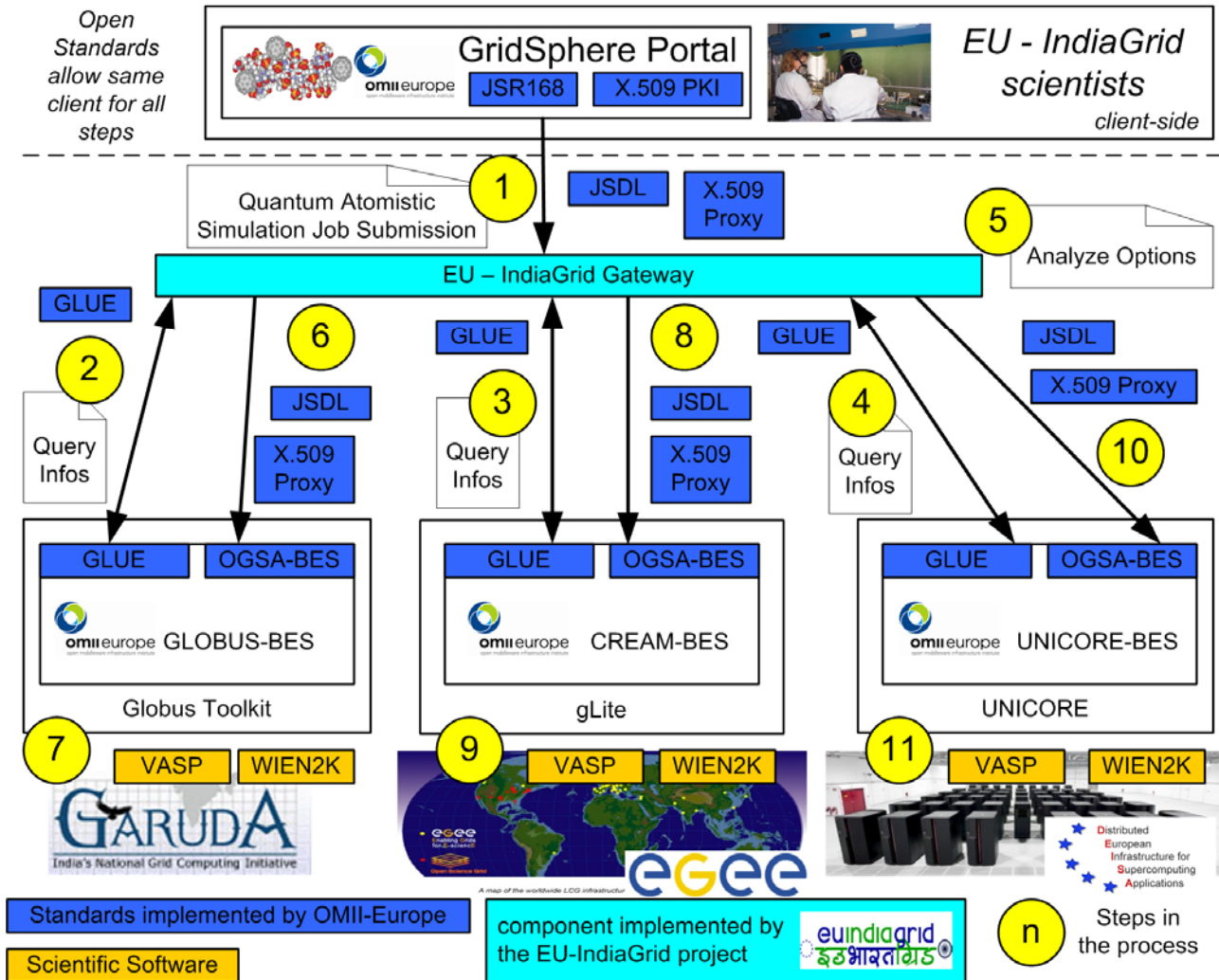
Step-wise description of interoperability scenario shown in overview

- Precondition: An EU-IndiaGrid e-Scientist is using the GridSphere portal and dedicated portlets within it that are JSR168 compliant and augmented with an **OGSA – Basic Execution Services (BES)** Web service (WS) client to interact with OGSA-BES compliant services. Also, the security setup is using the X.509 proxy standard, which is implemented in all systems in the scenario.
- **Step 1:** By using the GridSphere portal, different types of scientific jobs that are described in the **Job Submission Description Language (JSDL)** format are submitted to the EU-IndiaGrid Gateway. All these jobs are quantum atomistic simulations that require different scales of computing power.
- **Step 2:** After receiving this jobs, the EU-IndiaGrid Gateway contacts the Globus-BES component deployed on the GARUDA Grid in order to request pieces of information about the available resources that are described by using the **Grid Laboratory Uniform Environment (GLUE)** schema. OMII-Europe augments all OGSA-BES components with GLUE-based information in their properties, so that these components provide GLUE-compliant information about the nature of their resources they provide access to (e.g. available CPUs, memory, interconnection of Grid resources, etc.).
- **Step 3:** The Gateway performs the same request for GLUE-based information at the CREAM-BES component of gLite that provides information about its underlying resource.
- **Step 4:** Finally, the Gateway also performs the same request for GLUE-based information at the UNICORE-BES component of UNICORE that consist of information about the large HPC platforms.
- **Step 5:** This GLUE-based information from the different infrastructures is then analyzed by the EU-IndiaGrid Gateway, which selects the appropriate Grid where to execute the scientific simulations based on the size of the systems (i.e. required amount of CPUs/memory available on one resource).
- **Step 6:** The EU-IndiaGrid Gateway is able to translate the requests coming from the scientists in three different submission request categories that taking the required scale of the computing systems into account. In step 6, jobs that have low-scale to medium-scale parallel requirements and are mostly serial, are submitted to GARUDA via the GLOBUS-BES component secured using X.509 proxies. The jobs are submitted via OGSA-BES calls using the JSDL format (i.e. `CreateActivity()`).
- **Step 7:** GLOBUS-BES uses the JSDL to run either the VASP or WIEN2K scientific package on the GARUDA infrastructure on low-scale HPC resources or low amounts of CPUs for serial usage. The result can be obtained from with the portal or using SSH.
- **Step 8:** In a similar manner as step 6, the EU-IndiaGrid Gateway submits JSDL-compliant jobs that have medium-scale parallel requirements or use high amounts of CPUs for serial usage, to the EGEE infrastructure via the CREAM-BES component.
- **Step 9:** CREAM-BES uses the JSDL to run VASP or WIEN2K similar like step 7.
- **Step 10:** Finally, the EU-IndiaGrid Gateway submits JSDL-compliant jobs similar as steps 6 or 8 that have large-scale parallel requirements to DEISA via the UNICORE-BES component.
- **Step 11:** UNICORE-BES uses the JSDL to run the VASP or WIEN2K as massively parallel jobs on the DEISA infrastructure and its large-scale parallel resources.



Overview

Open Standards allow same client for all steps



Disclaimer

- This scenario describes a technical interoperability between Globus Toolkit, gLite and UNICORE enabled by the OMII-Europe project and thus the usage of GARUDA, EGEE and DEISA as described above is still subject to the scientists to negotiate with the respective infrastructures.

Links

- UNICORE Grid Middleware, <http://www.unicore.eu>
- gLite Grid Middleware, <http://glite.web.cern.ch/glite/>
- Globus Grid Middleware, <http://www.globus.org>
- OGF JSDL, <http://www.ogf.org/documents/GFD.56.pdf>
- OGF OGSA-BES, <http://www.ogf.org/documents/GFD.108.pdf>
- OGF GLUE, <https://forge.gridforum.org/sf/projects/glue-wg>

UNICORE

