Fact-Sheet WISDOM 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

- e-Infrastructure Islands in Europe: DEISA and EGEE
- Distributed European Infrastructure for Supercomputing Applications (DEISA)
  - Supercomputing / High Performance Computing (HPC) Community
  - 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)
  - Grid suitable for massively parallel scientific jobs (MPI, OpenMP, etc.)
- Enabling Grids for e-Science (EGEE)
  - Mainly High Energy Physics (HEP) community and other communities
  - 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
  - Grid suitable for embarrassingly parallel scientific jobs
- Both Grids are in 2007 not technically interoperable and had less adoption of standards in the past

Requirements of Wide In Silico Docking on Malaria (WISDOM) Project

- WISDOM aims at developing new drugs for Malaria, Link: http://wisdom.eu-egee.fr/
- WISDOM uses EGEE for large-scale in silicio docking
- e-Scientists use a computational method for prediction whether one molecule will bind to another
  - Using the Autodock and FlexX software provided via gLite in EGEE
  - Output is a list of best chemical compounds: But only potential drugs, not the final solution
- Idea: Refine best compound list via molecular dynamics (MD)
  - Final solution is currently computed in EGEE, but could be done more efficiently in DEISA
  - Fast MD computations could use the scalable AMBER code within DEISA
  - Assisted Model Building with Energy Refinement (AMBER), deployed in DEISA in Version 9
- **GOAL: Accelerate drug discovery with EGEE and DEISA using OMII-Europe components**

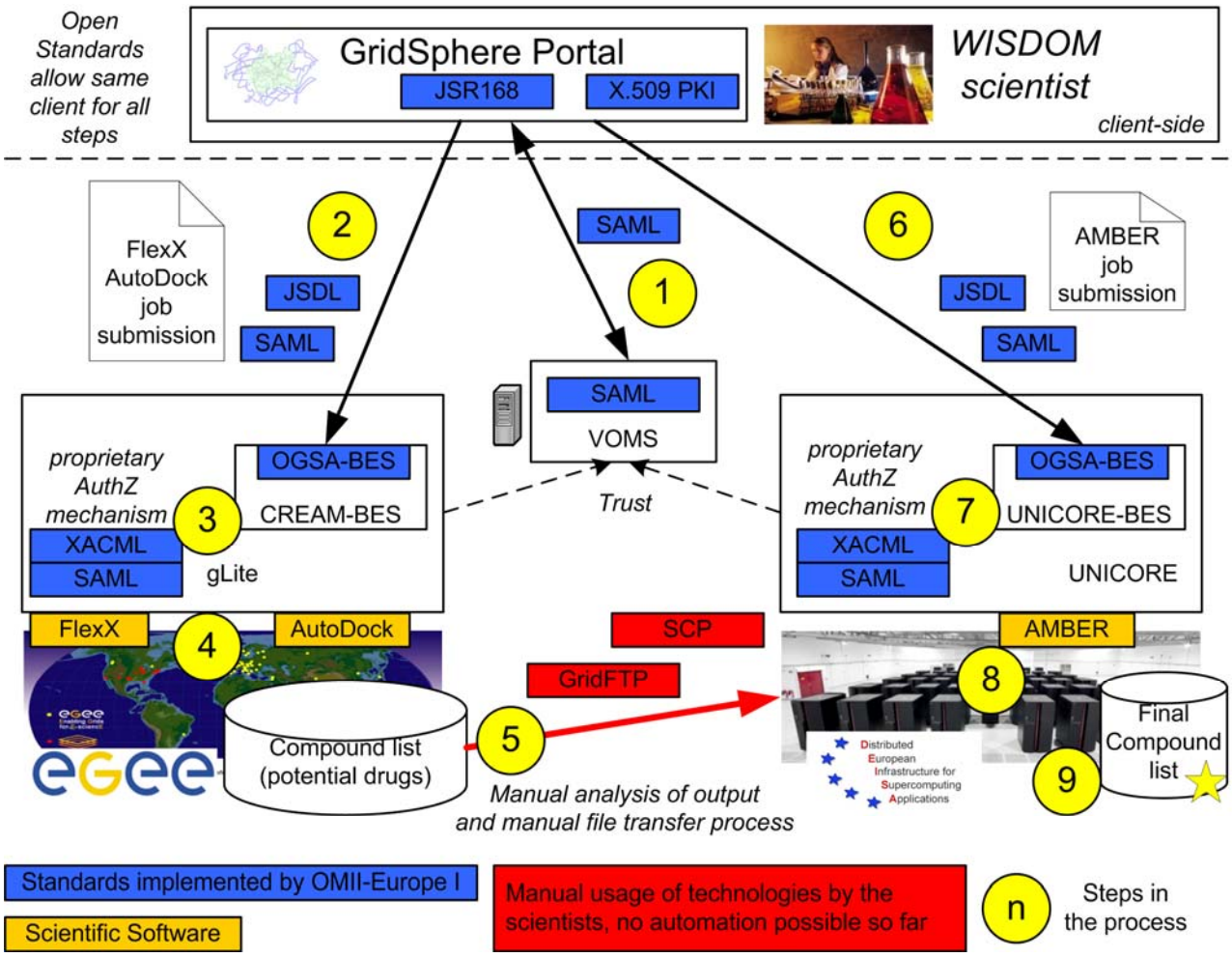
´Description of interoperability scenario

- This interoperability scenario is a demonstrator of how WISDOM e-Scientists can use both infrastructures EGEE and DEISA to improve their daily work
- This scenario represents a whole class of similar interoperability scenarios with similar requirements for interoperability between EGEE and DEISA
- It shows how OMII-Europe components are used to enable interoperability between upcoming standard-compliant versions of UNICORE 6 and gLite that might be deployed in the e-Infrastructure EGEE and DEISA soon.

Step-wise description of interoperability scenario shown in overview

- Precondition: A WISDOM e-Scientists 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.
- **Step 1:** By using the GridSphere portal a Web service callout is started to the new **Security Assertion Markup Language (SAML)-based Virtual Organization Membership Service (VOMS)** that releases signed SAML assertions stating the identification and role possession of the WISDOM scientist.
- **Step 2:** After receiving the SAML assertion it is used by the portal to access the OGSA-BES compliant CREAM-BES service of gLite. This Web service callout also includes a job description compliant with the **Job Submission Description Language (JSDL)** describing the start of the FleXX and/or AutoDock applications via gLite on the EGEE infrastructure.
- **Step 3:** As part of gLite in the near future, the CREAM-BES service is using the JSDL document to invoke the FleXX and/or AutoDock applications via gLite, including parameters written in JSDL. Before both can be finally started on the infrastructure, an authorization of the scientific JSDL job must be performed by using the SAML assertion in conjunction with proprietary authorization systems so far. This in fact is a particular potential for OMII-Europe 2 to implement a common authorization service that may be based on the **Extensible Access Control Markup Language (XACML)** standard.
- **Step 4:** FleXX and/or AutoDock are computed on the EGEE infrastructure as embarrassingly parallel scientific applications. The outcome of this job is an intermediary result in terms of a compound list that represents potential drugs.
- **Step 5:** To use these intermediary results of the EGEE job outcome within the DEISA infrastructure, the data must be transferred to DEISA storage systems. This can be done manually using GridFTP or SCP since these steps required a manual intervention from the scientist. Hence, the scientific process requires that scientists analyze the outcome of the EGEE jobs and take particular ones as input for the DEISA jobs. Therefore, a manual transfer process is not a problem here so far. However, it would be more convenient for scientists if this could be done via Grid middleware directly.
- **Step 6**: Assuming that the data of the intermediary results are reachable within DEISA, the WISDOM e-Scientists use again the portal to submit another JSDL-compliant job to the UNICORE OGSA-BES interface implementation. This time the JSDL describes the highly scalable AMBER library c/fortran code execution within DEISA. Again, the (not necessarily same) SAML assertion must be transferred during this WS call to ensure the authorization of the scientist later within UNICORE.
- **Step 7**: As part of UNICORE 6 in the near future, the UNICORE-BES service is using the JSDL document to invoke the AMBER application via UNICORE, including parameters written in JSDL. Before this application can be finally started on the DEISA infrastructure, an authorization of the scientific JSDL job must be performed by using SAML assertions in conjunction with proprietary authorization systems. Similar to Step 3, this can be also achieved in a more standard-compliant way by standards that might be provided by OMII-Europe 2 if funded.
- **Step 8**: The AMBER application is computed on the DEISA infrastructure as massively parallel scientific application. This step is now significantly faster than without the interoperability between EGEE and DEISA, because the AMBER code is highly scalable and thus capable of leveraging the massive amounts of CPUs available in DEISA. The outcome of this job is the final result.
- **Step 9**: Finally, by using UNICORE on DEISA the outcome of this job, which is the final compound list can be obtained. All in all, the solution has been computed within EGEE and DEISA.

Overview



Disclaimer

- This scenario describes a technical interoperability between gLite and UNICORE enabled by the OMII-Europe 1 project and thus the usage of DEISA and EGEE 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/
- OGF JSDL, http://www.ogf.org/documents/GFD.56.pdf
- OGF OGSA-BES, http://www.ogf.org/documents/GFD.108.pdf
- OASIS SAML, www.oasis-open.org/committees/security/
- OASIS XACML, www.oasis-open.org/committees/xacml/