



A Grid Workflow Management System

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Outline

- Grid WorkFlow Management System

- ProGenGrid WFMS
 - Editor
 - Meta Scheduler

- Conclusions and Future Work

Grid WFMS

- ***Grid Workflow Management System (WFMS)*** specifies complex (distributed) applications, integrating and composing individual simple services:
 - *Workflow definition* through a formal description (Editor);
 - *Workflow execution (Meta Scheduler)* responsible of the enactments, by controlling and coordinating execution of applications..

Workflow ProGenGrid

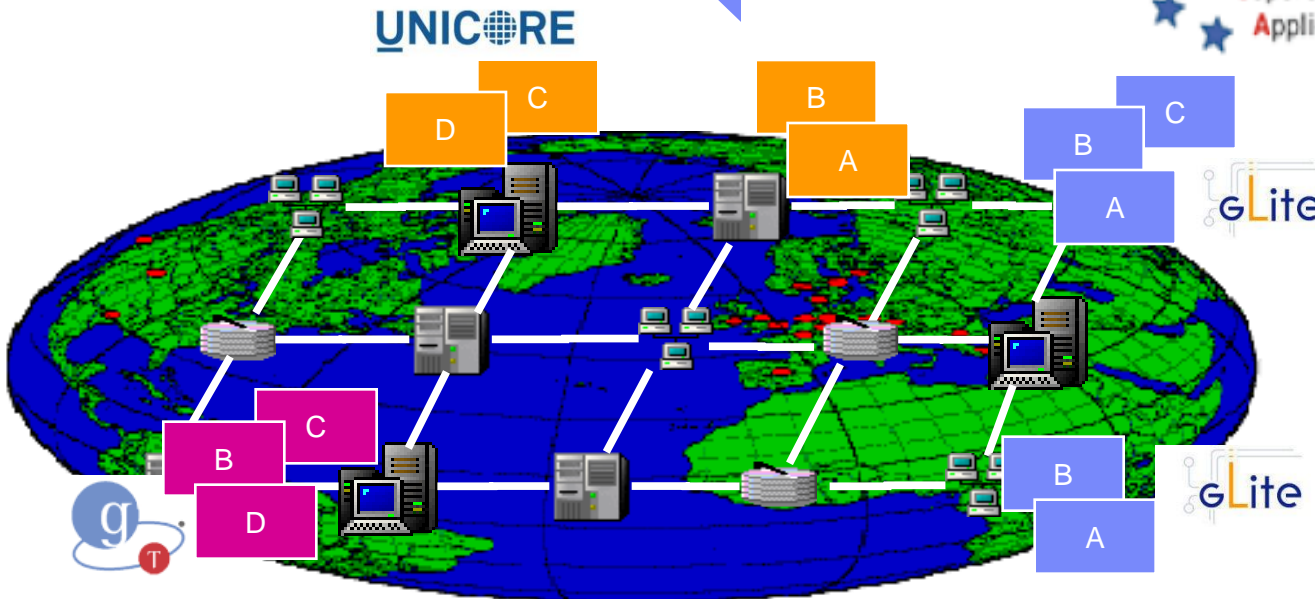
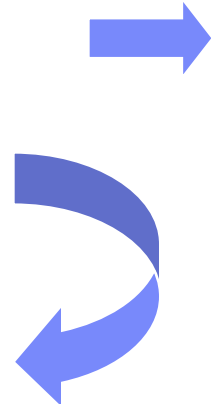
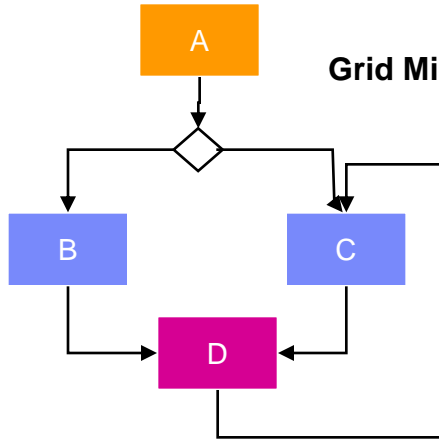
- **Proteomics and Genomics Grid Project** (started in the 2004): aims at building a Grid Problem Solving Environment for the simulation of the complex experiment in Bioinformatics.
 - The results of this project are used in the LIBI (International Laboratory of Bioinformatics), 2005-2010.



- See Talk in the Grid Projects and Collaborations Session (March 5, 2009)
- **Goal:** Plan and Development of a WFMS for composing applications, run on computational resources of different Grid middleware such as gLite, Unicore and Globus.

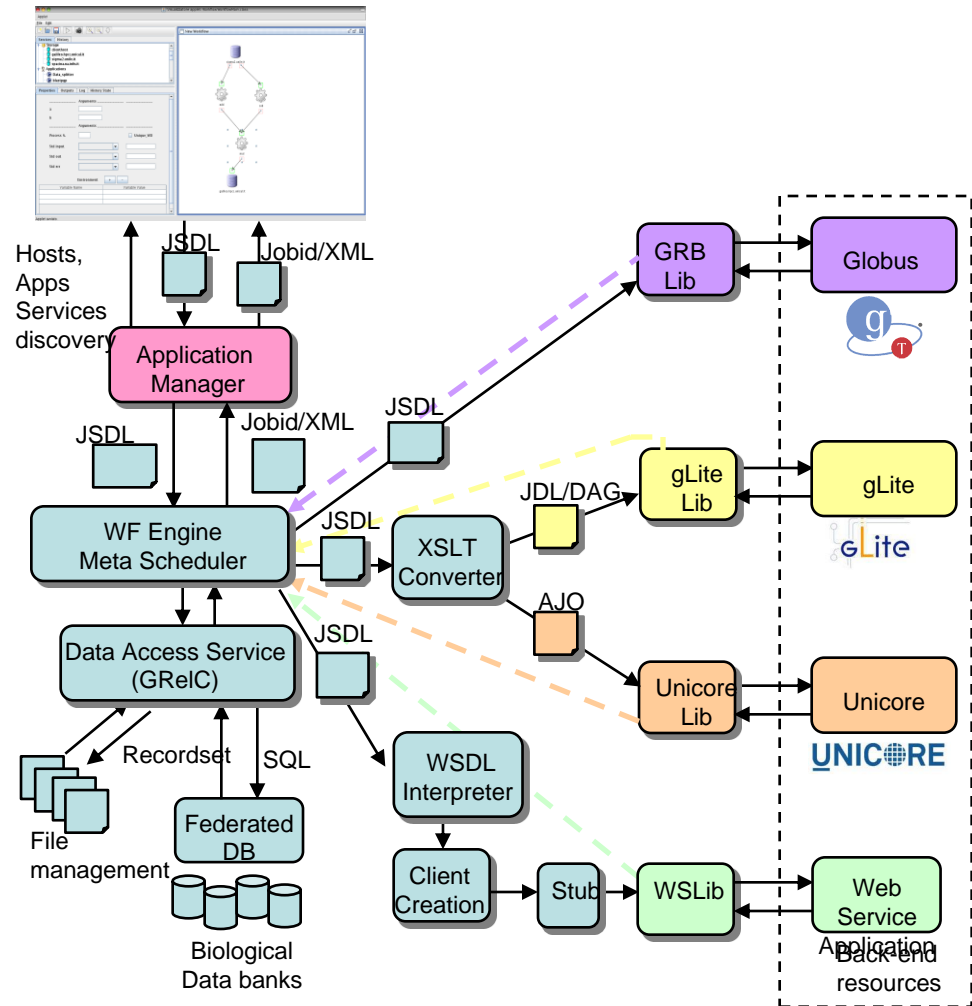
Scenario

Grid Middleware: Interoperability - the Big Issue



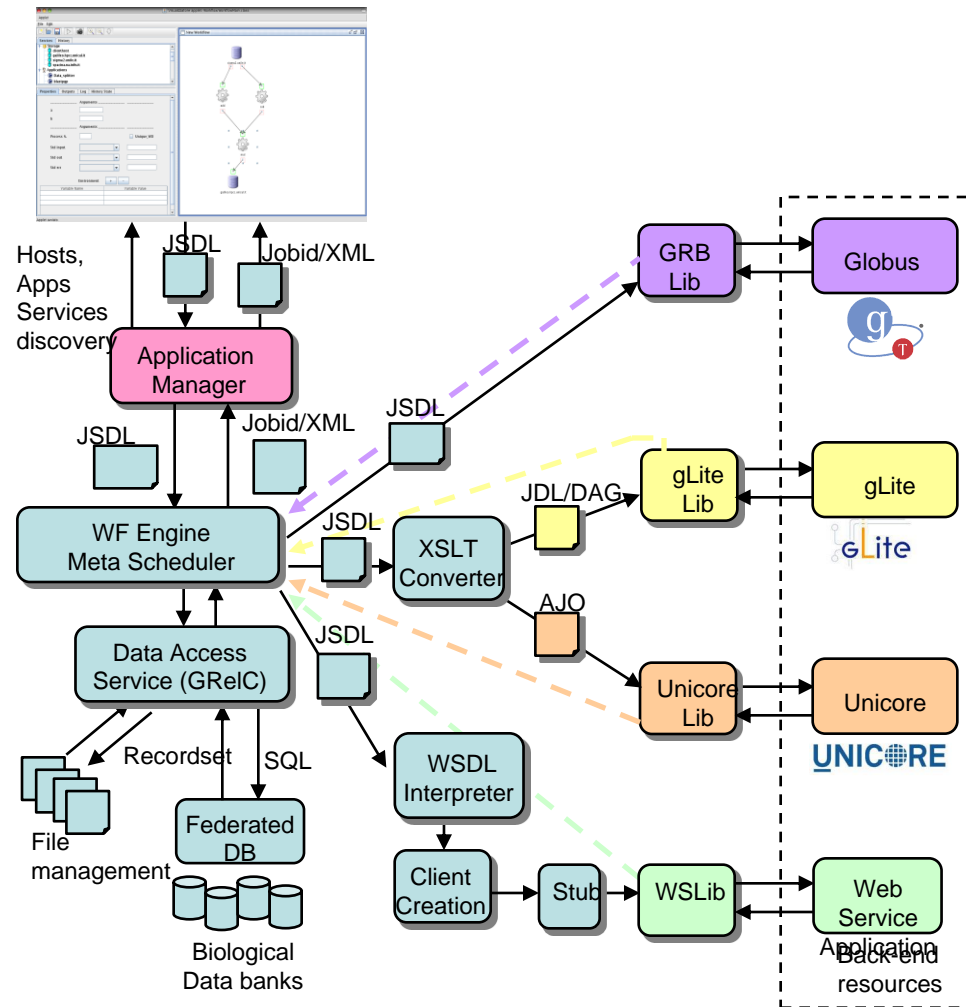
ProGenGrid WFMS Architecture

- Editor
- Application Manager
- WF Engine Meta Scheduler
 - GRB_Lib
 - gLite_Lib
 - Unicore_Lib
- GReIC DAIS □



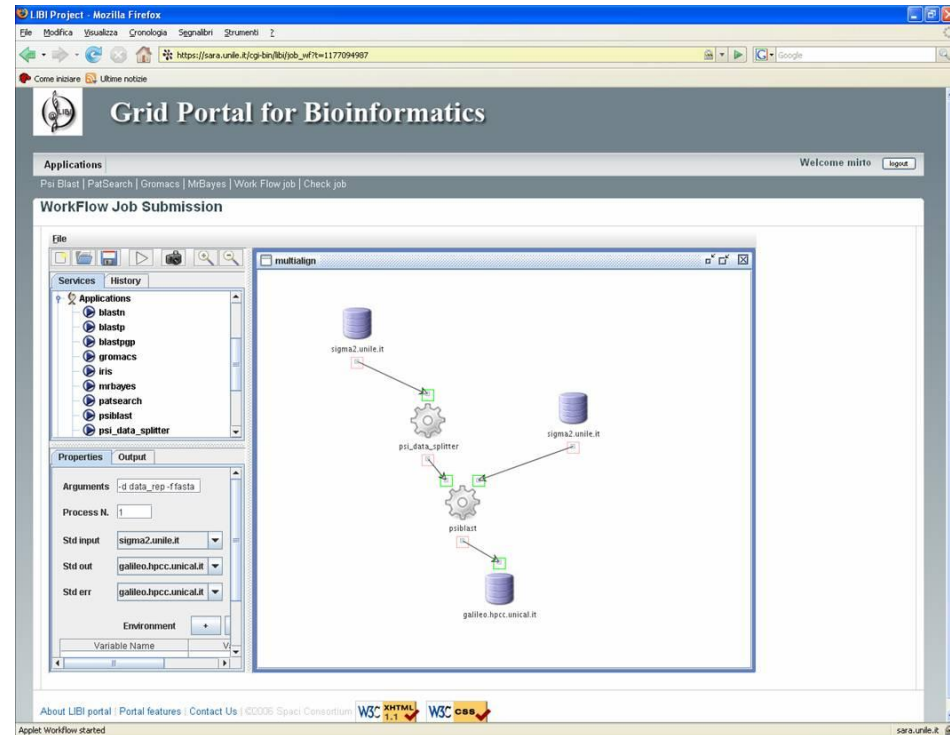
Grid WFMS

- ❑ First release of the ProGenGrid WF
 - client-server;
- ❑ Second release
 - GRB Web Service Engine for supporting Globus based jobs
 - batch, parameter sweep, MPI jobs.
- ❑ Current release (work in progress)
 - Meta scheduler for the cooperation of the Globus, Unicore and gLite middleware.



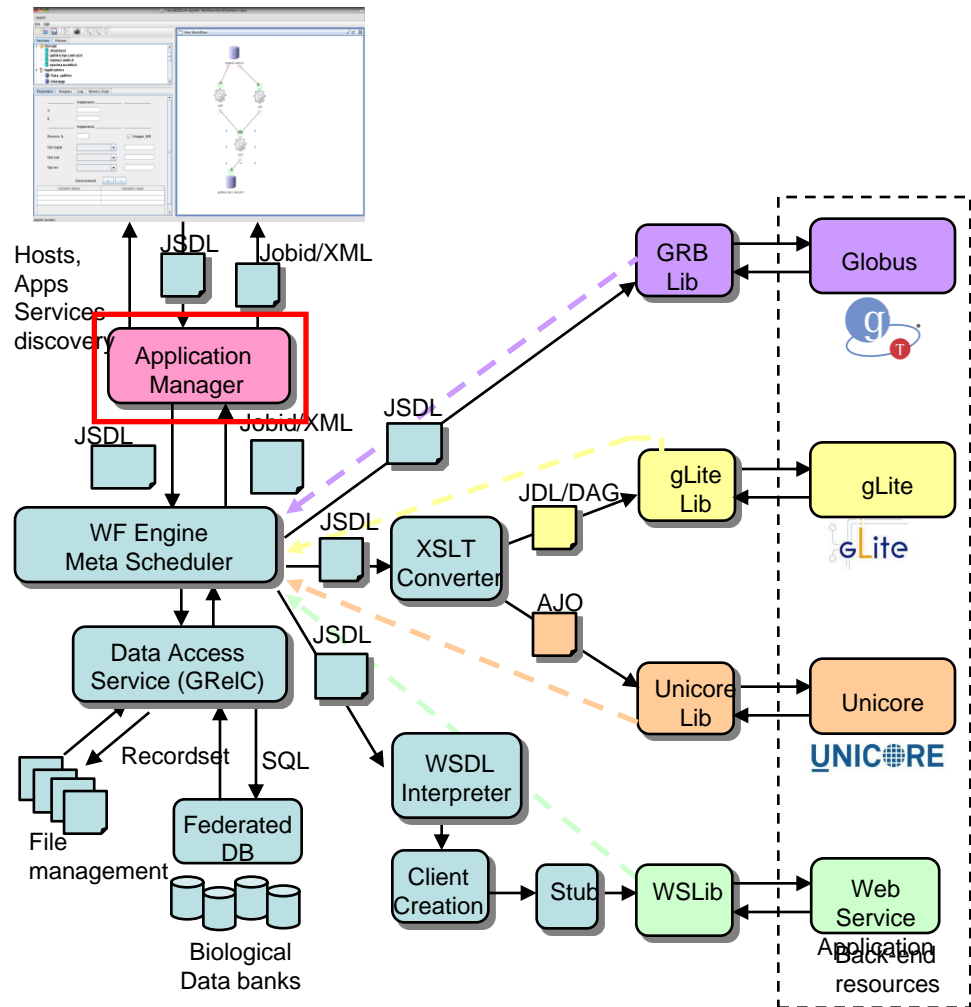
Editor

- Workflow described as graph:
 - DAG (Directed Acyclic Graph)
 - DCG (Directed Cyclic Graph)
- Features:
 - Resources, Host and Services discovery;
 - Composition of the graph by using drag and drop;
 - Specification of the arguments related to each application;
 - Stage-in and Stage out from repositories;
- Implementation as signed Java applet:
 - Access at the filesystem of the client;
 - Exchange of data and messages with the server.



Application Manager

- ❑ Handle User account and application profile;
- ❑ Check data consistency;
- ❑ Build JSDL (Job Submission Description Language)
 - Compliant OGF standard
- ❑ Produces two file:
 - View XML (Abstract WF)
 - JSDL XML (Concrete WF)



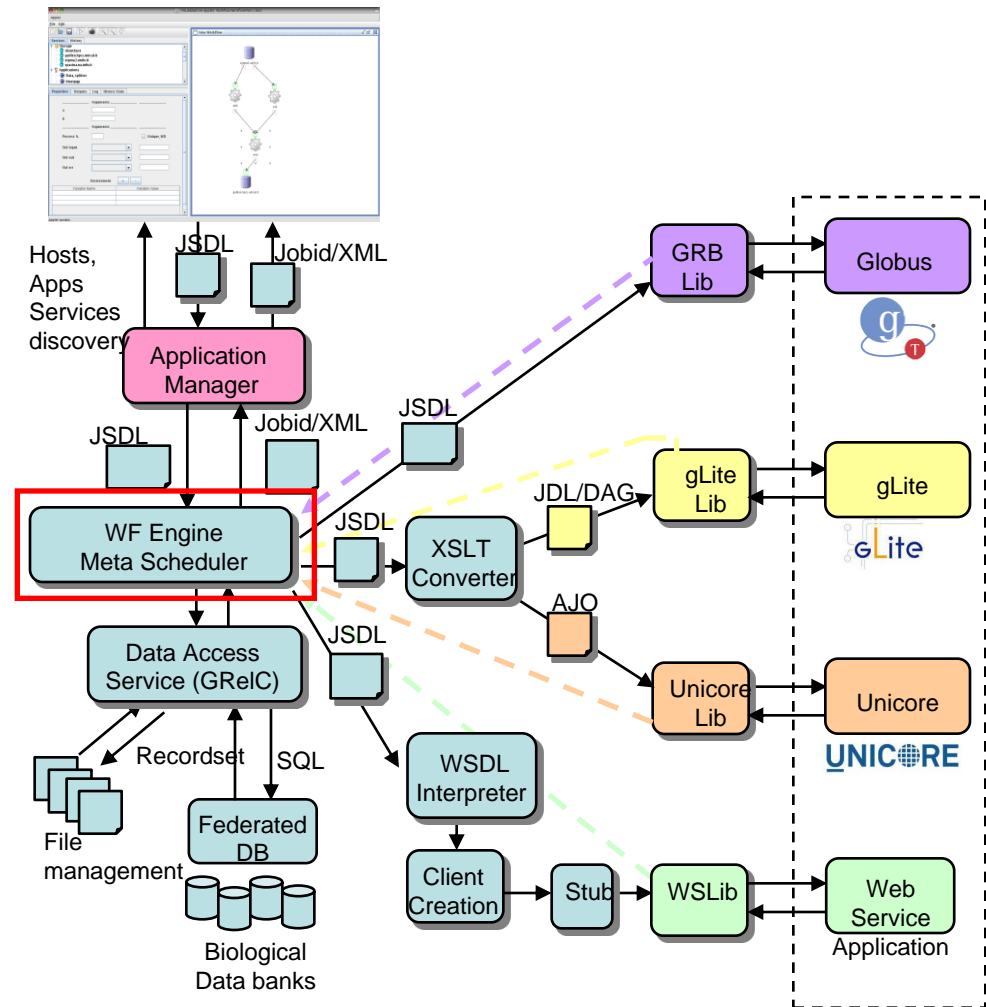
WF Engine - Meta Scheduler

It handles both

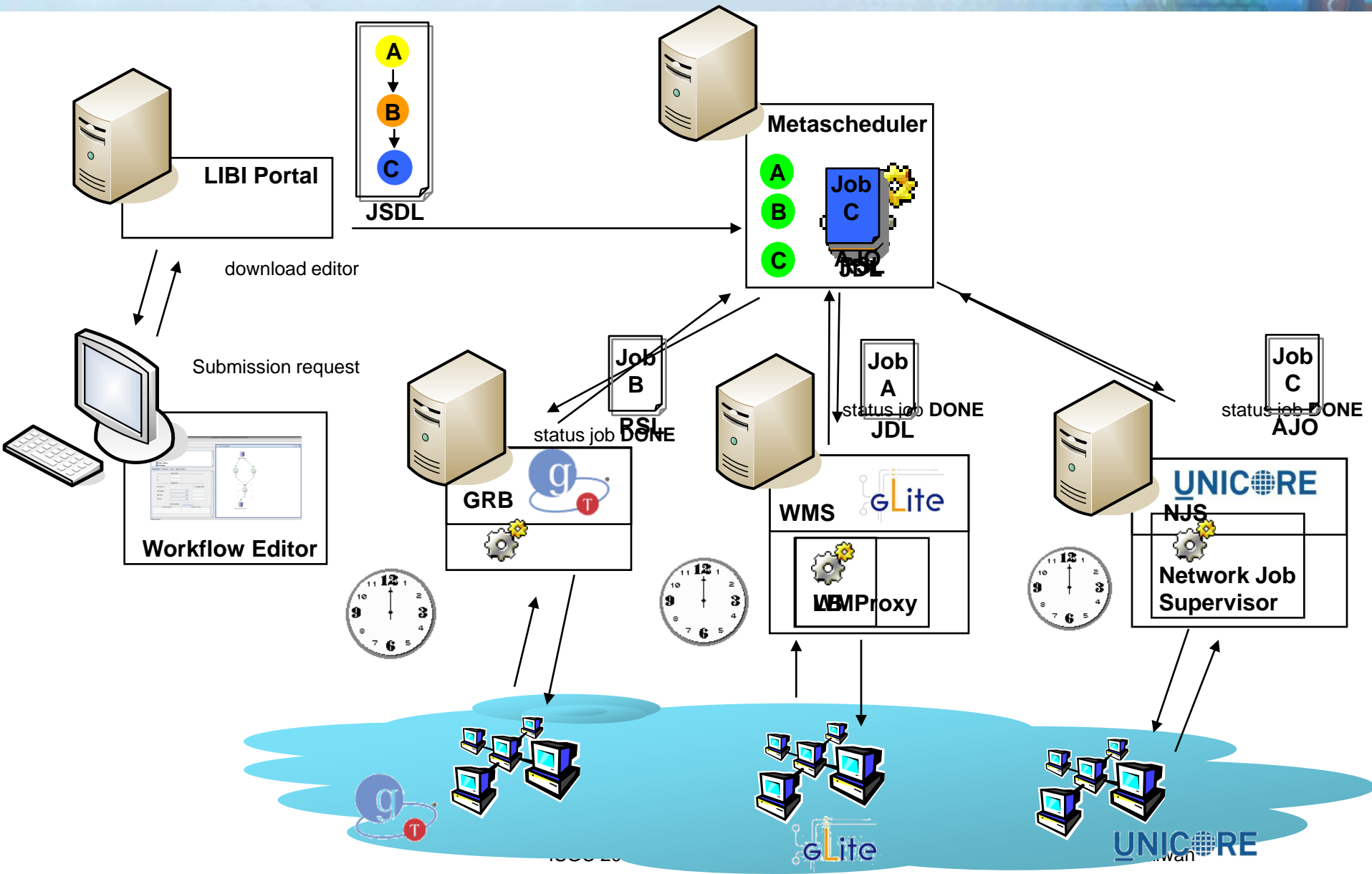
- simple workflows described by DAGs;
- complex workflows described by arbitrary graphs, supporting cycles and conditions;

It supports for recursive composition i.e., the possibility to define a workflow vertex as a sub-workflow or parameter sweep vertex instead of a batch task;

Workflow engine implements a dynamic scheduling policy leveraging the parallelism inside the graph.



WFMS in action



Issues in the interoperability with gLite, Unicore, Globus

- ❑ **We have considered several sources of heterogeneity:**
 - *Language*
 - *Job Submission*
 - *Job Support*

Language

- ❑ **RSL** (*Resource Specification Language*) for Globus;
- ❑ **JDL** (*Job Description Language*) for gLite;
- ❑ **AJO** (*Abstract Job Object*) for Unicore.

We considered an extended **JSDL** language, to invoke remote and local services and pass results between them.

JSDL adds resource requirements and data staging. It is translated by the Meta Scheduler in the opportune language by using several adaptors.

Job submission

❑ Globus

- Using RSL we can define once the file to be staged in, **executed** and staged out. The file transfer is made by GRAM

❑ gLite

- The job is specified through a JDL description this can include references to remote files to be staged in or staged out from SE
- The files must be present in the SE before job starting. The file transfer must be made explicitly by the client through a gridftp session

❑ UNICORE

- The job is specified through an AJO object
- A single AJO does not contain references to remote files to be transferred
- The stage in or stage out phase must be made explicitly by the client submitting a job for file transfer

❑ Meta scheduler Job Submission:

- Stage in of needed input files
- Stage in of the executable
- Job execution
- Stage out of produced output files

Job support

Globus

- Does not support parameter sweep nor workflow job

gLite

- Supports job array, workflow job (only DAG), batch job

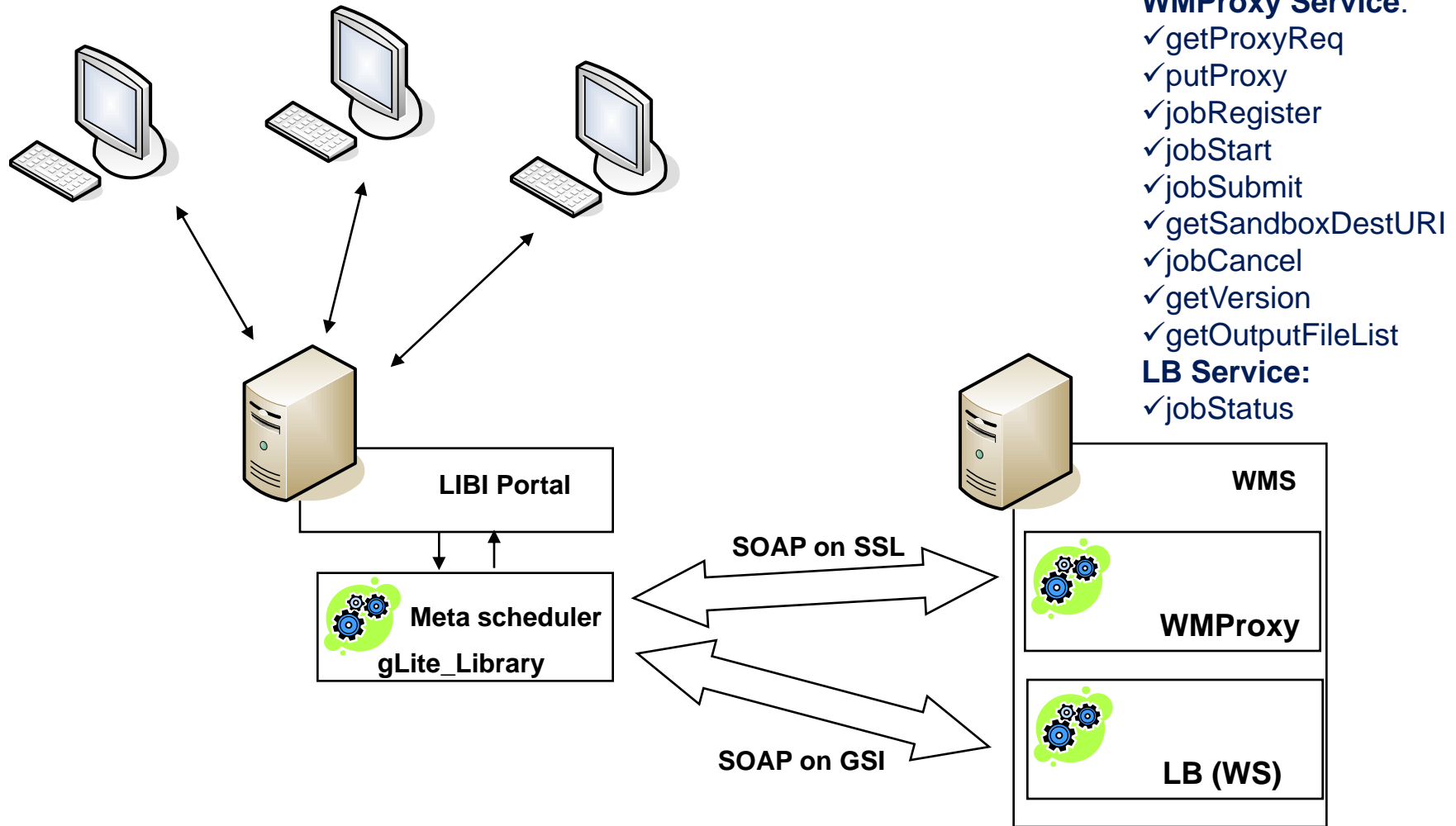
UNICORE

- Does not support parameter sweep jobs

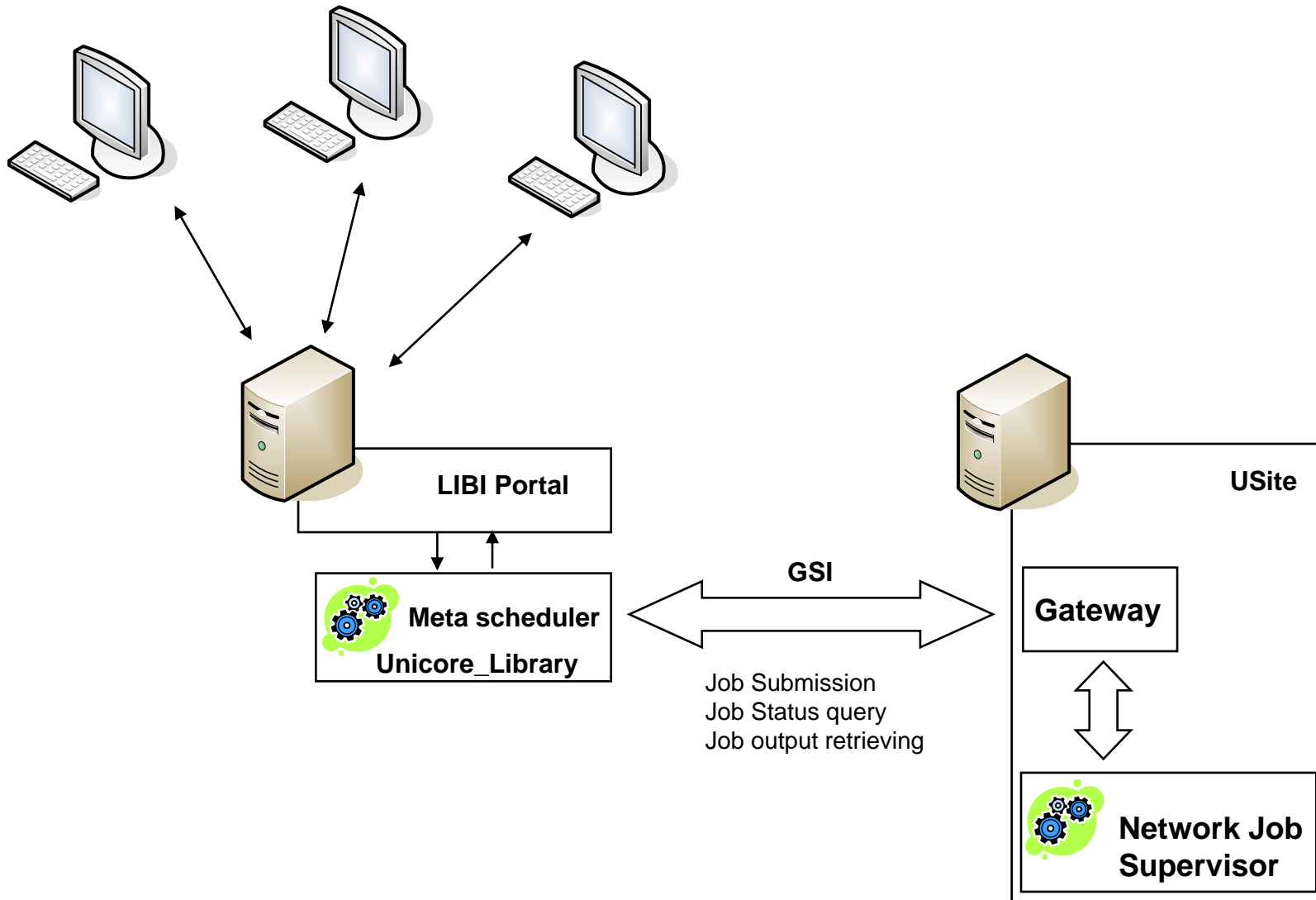
Meta scheduler job types:

- Single batch: synchronous and asynchronous
- Parameter sweep job
- Workflow job

gLite_Lib: WS clients to the gLite middleware



Unicore_Lib: a client for the Unicore middleware



GReIC DAIS

- ❑ The access to the data is carried out through the GReIC DAIS;
- ❑ It is a WS component and the needed information such as the service access url, input query (in SQL format) are specified in the JSDL file;
- ❑ In the Editor, GReIC DAS client is a task;
- ❑ JSDL is parsed by the engine that contacts the service and retrieves the data;
- ❑ Within the LIBI project, the access in grid to the LIBI Federated DB is carried out through the GReIC DAIS. Two complementary layers:
 - the LIBI federator server performs the data federation task of about 10 heterogeneous and distributed data sources such as UTRef, MitoRes, UTRSite, GenBank, OMIM, Pubmed, EMBL, HmtDB, Uniprot,EMBL_CDS;
 - the GReIC DAIS exposes the federated DB in grid making it available to all of the LIBI grid users.

Conclusions and Future Work

- ❑ We have reported the recent advances related to the ProGenGrid Workflow Management System;
- ❑ In particular, we have described the architecture of the workflow engine meta scheduler, which now allows the interoperability with different grid middlewares and Web Services applications.

Future work:

- ❑ Full deployment of the Meta Scheduler in June and related testbed on real bioinformatics case studies in the LIBI Project
 - Tertiary structure prediction and phylogenetic bayesian analysis;
- ❑ Development of a plugin for the support to the CREAM service of gLite;
- ❑ Development of the jobs monitoring into the GUI;
- ❑ Supporting GRelC task in the WF for retrieving data needed to the applications.

Contacts

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Questions

