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Interoperation of world-wide production e-Science infrastructures

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Open Grid Forum—Grid Interoperation Now (GIN)—Community Group (CG)

SUMMARY

Many production Grid and e-Science infrastructures have begun to offer services to end-users during the past several years with an increasing number of scientific applications that require access to a wide variety of resources and services in multiple Grids. Therefore, the Grid Interoperation Now—Community Group of the Open Grid Forum—organizes and manages interoperation efforts among those production Grid infrastructures to reach the goal of a world-wide Grid vision on a technical level in the near future. This contribution highlights fundamental approaches of the group and discusses open standards in the context of production e-Science infrastructures. Copyright © 2009 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Many Grid projects have begun to offer production services to end-users during the past several years. While many end-users are satisfied with the resources and technology provided within these infrastructures, there are also an increasing number of application projects that require access to a wide variety of resources and services in multiple Grids. The requirements for such a wide variety of resources begin with small PC pools and expand to medium-sized clusters and large-scale high-performance computing (HPC) resources. One well-known reason for these different requirements, among others, is an increasing complexity of Grid applications that embrace multiple physical models (i.e. multi-physics) that consider a larger range of scales (i.e. multi-scale). Implementations of such models create a steadily growing demand for compute power as well as storage capacities. Hence, collaboration across typical physical knowledge boundaries leads to totally new complex scientific physical models that have to be simulated on different Grid resources within those infrastructures, which will thus face new challenges during the coming years.

Also, more and more world-wide scientific domain-specific Grid infrastructures emerge orthogonal to national Grid initiatives. While both Grids have experts in the respective scientific communities, the technology used in those Grids is typically not interoperable with each other due to their historic evolutions or funding models. Hence, the collaboration between these Grids is difficult and could be significantly improved. Other requirements for interoperability are based on the demand for usage models of different services that are available in different Grid infrastructures. Apart from scientific domain-specific services, there are even more general diverse services available in Grids. To provide one example, while some Grids provide brokering mechanisms to automatically choose available Grid resources, other Grids fundamentally require that Grid resources have to be manually chosen from e-Scientists to satisfy their unique requirements.

All in all, there are more and more requirements and demands for interoperation of production Grid and e-Science infrastructures emerging today. Even if many scientific applications from various domains have already taken advantage of these infrastructures in the past, new possibilities based on a real interoperation of Grids will lead to even more new insights during scientific scenarios. Therefore, the purpose of the *Grid Interoperation Now* (GIN) *Community Group* (CG) [1] of the *Open Grid Forum* (OGF) is to organize, manage and demonstrate a set of interoperation efforts among such production infrastructures. The members of the GIN–CG are representatives of world-wide Grid and e-Science infrastructures and national Grid initiatives, all working on a technical level to achieve the compelling vision of a true global Grid.

Within this contribution, we define the difference between *interoperation* and *interoperability* as follows. Interoperation is specifically defined as what needs to be done to get production Grids to work together as a fast *short-term achievement* using as much existing technologies as available today. Hence, this is not the perfect solution and relies on workarounds or tweaks of technologies that only last as long as there is no fundamentally new version of the technology available. Thus, interoperation is much different than interoperability, which is herein defined as the native ability

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of Grids and Grid technologies to interact directly via common open standards in the future. We will discuss within the contribution why this is a rather *long-term achievement* and why early interoperation success stories have to use short-term achievements.

The contribution of this paper to the overall work in the field of interoperability and interoperation within the e-Science and Grid communities is that GIN provides newly developed components and adapters that work today and include efforts within the most known production Grid and e-Science infrastructures. Hence, this paper basically describes various approaches that enable e-Scientists to work in more than one production Grid tomorrow if they want to. The efforts to achieve this is an outcome of different working areas within GIN such as job submission, data management, security setups and information exchange.

Finally, it is important to mention that the GIN effort does not include any attempt to provide a common allocation or brokering of resources between production Grid projects and infrastructures. This is viewed as beyond the scope of the GIN efforts and resource allocation decisions are left to negotiations between projects, e-Scientists and the individual Grid infrastructures. In collaboration with GIN, the recently started OGF-Europe project maybe able to make a significant step forward in this context. Nevertheless, the work within GIN demonstrates that interoperation is feasible and technically possible today; thus, basically enabling e-Scientists to work on cross-Grid scenarios and applications that need more than one Grid for their scientific research.

This paper is structured as follows. After the motivation and introduction into the problem domain of interoperation and interoperability, Section 2 shortly introduces the GIN–CG and its participating Grid infrastructures. Section 3 provides an overview of the wide variety of GIN efforts. It describes the fundamental process of providing a cross-Grid information system, job submissions, data management, security setups and outlines potential solutions. This section also includes some information on the well-known Supercomputing 2006 and 2007 demonstrations. In Section 4, we provide lessons learned from these demonstrations and provide some insights to a very interesting session at OGF21 that brought together GIN, software providers as well as standardization groups. In this section, we also provide the current status of standard adoption within GIN infrastructures as discussed at OGF22. Finally, this paper ends with a survey of related work and concluding remarks.

2. GRID INTEROPERATION NOW COMMUNITY GROUP

The origin of the GIN group began in November 2005 when Charlie Catlett organized a multi-Grid interoperation planning meeting with well-known representatives from world-wide Grid infrastructures. The results of this meeting basically lead to the GIN group with a slightly different focus than today. Initially, the scope of GIN was to pursue interoperation on 6–8 month horizons using solutions for which there are working implementations available, wherever possible using open standards. The results of GIN were expected to lead to a more seamless usage of different Grid infrastructures by applications although GIN did not provide resources or support application porting. Also today, GIN provides a seamless usage of different Grid infrastructures on the technical level, but real usage is still required to negotiate between end-users, resource providers and Grid infrastructures.

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Table I. Grid and e-Science Infrastructures participating in GIN.

Name	Country/Continent/Region
APAC	Australia
D-Grid	Germany
DEISA	Europe
EGEE	Europe
NAREGI	Japan
NDGF	Nordic Region
NGS	U.K.
OSG	U.S.A.
PRAGMA	Pacific Region
TeraGrid	U.S.A.

More recently, the goals of GIN are to organize, manage and demonstrate interoperation between production Grid infrastructures. GIN provides valuable feedback to the OGF standardization groups and the software providers implementing those standards in technologies that are deployed on the infrastructures. Also, if required, GIN works closely with important activities that focus on special areas, such as the *Grid Laboratory Uniform Environment* (GLUE) [2] group or the new spin-off activity focusing on *worker node profiles*.

All Grid infrastructures that participate within GIN are shown in Table I. There are several national Grid activities participating such as the *Australian Partnership for Advanced Computing* (APAC) [3], the German national Grid initiative *D-Grid* [4], or the Japanese *National Research Grid Initiative* (NAREGI) [5], or the *National Grid Service* (NGS) [6] within the U.K. The European participating infrastructures are *Enabling Grids for e-Science* (EGEE) [7] and the *Distributed European Infrastructure for Supercomputing Applications* (DEISA) [8]. Also, several regional Grids participate such as *Pacific Rim Applications and Grid Middleware Assembly* (PRAGMA) [9], *Nordic DataGrid Facility* (NDGF) [10]. Finally, participating Grids from U.S.A. are *TeraGrid* [11] and the *Open Science Grid* (OSG) [12].

To achieve real usable interoperation, GIN implements interoperation in five specific areas. First, *authorization and identity management* (GIN-AUTH) deals with resource sharing among members of the GIN Virtual Organization (VO) [13]. Second, the *data management and movement* (GIN-DATA) area is working on the interoperation of different data management technologies currently in use of multiple e-Science infrastructures. These include the Storage Resource Broker (SRB) [14], Storage Resource Managers (SRM) [15] and GridFTP [16]. Third, the *job description and submission* (GIN-JOBS) area focuses on job management across different Grid technologies and middlewares used in production Grids today. In addition, tracking the resource usage of these submissions is especially interesting in cross-Grid scenarios and thus also part of this area. Also important for end-users is the *information services and schema* (GIN-INFO) area, because the efforts conducted in this area basically provide the base for cross-Grid interoperation taking up-to-date information into account. These interoperations rely on information models such as *Common Information Model* (CIM) [17] and GLUE [2], and on information systems such as *Berkeley Database Information Index* (BDII) [18] and *Monitoring and Discovery Services* (MDS) [19]. Finally, the *pilot test applications* (GIN-OPS) for cross-Grid operations use different applications that require resources from multiple Grid infrastructures.

3. GIN ACTIVITIES

The major GIN activities are related to the organization and demonstration of technical interoperation between production Grid infrastructures. As described earlier, we define interoperation different from interoperability; however, it seems very reasonable to consider both approaches in the GIN efforts since they are closely related. In fact, many of the rather short-term interoperations should lead to long-term open standards-based interoperability in the near to mid-term future. Therefore, all GIN efforts can be not only differentiated into the different areas (i.e. GIN-JOBS, GIN-AUTH, etc.), but also in two categories named as *production* and *future solution*.

Thus, many approaches undertaken in GIN are part of the production category, which includes efforts having the short-term interoperation character. In this category, we refer to non standard-based solutions for which there are working implementations available, even if they are realized by using workarounds, adapters, tweaks or even small hacks. On the other hand, approaches of the future solutions category use open standards (i.e. OGSA-BES [20]) where possible. This might even include emerging standards (i.e. OGSA-RUS [21]) that are still not yet an official open standard, but have a high potential to be standardized in the near future and are urgently needed within the infrastructures.

In this chapter, we provide an overview of the undertaken GIN efforts from 2006 until today in the following paragraphs. Most notably, these efforts include the well-known demonstrations as presented in media [22] and shown at Supercomputing 2006 in Tampa and the more recent Supercomputing 2007 in Reno. Typically these efforts are achieved in many different projects while GIN provides them a forum for discussions and exchange of experience in interoperability and interoperation. Hence, many demonstrations are organized by GIN, but having much contributions from a wide variety of world-wide Grid projects.

Finally, lessons learned based on the efforts described in the following paragraphs are presented later in Chapter 4.

3.1. Information services and modeling

In order to identify appropriate resources for end-users within an e-Science infrastructure, there must be some form of *resource information conforming to schemas* and *access technologies with standard query mechanisms*. The GIN-INFO area of GIN provides interoperation components (e.g. information schema translators, adapters, etc.) to deal with access to different information schemas within production e-Science infrastructures. The efforts in the GIN-INFO area are built upon previous bi-lateral successes such as interoperation efforts between EGEE and OSG, and between NDGF and EGEE, and others. Hence, the major goal of GIN-INFO is to extend these pair-wise interoperations with a broader set of production Grids by identifying a subset of information items that can be used as a *common minimum set*. This also motivates the development of translators for common information items used in different information schemas.

Information systems describe the wide variety of Grid resources that are available in production Grids in a precise and systematic manner, to enable them to be discovered for subsequent management or use. Over the years several schemas evolved either in scientific-oriented production Grids or within business-oriented standard bodies such as the *Distributed Management Task Force (*DMTF*)*. Figure 1 illustrates the initial architecture of the BDII-based interoperation between

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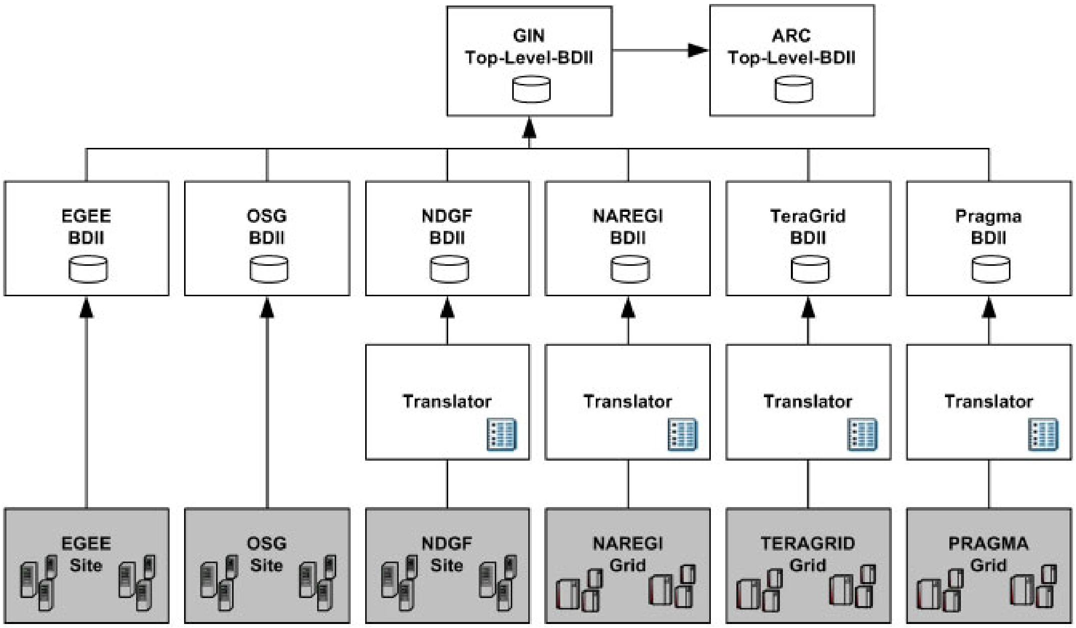

Figure 1. Information schema translators for production Grid interoperations.

different information services and schemas. BDII itself consists of two or more standard LDAP [23] databases that are populated by an update process. The update process obtains data encoded in LDIF [24] either by doing an ldapsearch on LDAP URL lists or by running a local script that generates LDIF. The LDIF is then inserted into the LDAP database as an entry.

Within GIN-INFO, we initially developed numerous information translators for those Grids that do not naturally support the BDII system. This raised a demand for a set of common minimal attributes, because the production Grids evolved over time and thus use a wide variety attributes that deal with more or less the same pieces of information. Therefore, in interoperation, it is extremely important to agree on a *common minimal set of attributes*. Of course this common minimal set depends on the use case: for instance, in job execution the service endpoint attributes may be published by an information system. In addition, to have a common minimal set of attributes it is necessary to map the values to each other so that clients are able to interpret attributes consistently. Hence, translators have been developed that map the content of one attribute in schema A to the content of one attribute (or even a set of attributes) in schema B. The translators are publicly available to be used within the Grid community.

As shown in Figure 1, we used a GIN-BDII as a top-level BDII with information (attributes) from all Grids in accordance to the GLUE schema version 1.3 [2]. As a side remark, this version of GLUE was created before the OGF GLUE working group was formed that currently develops the GLUE 2.0 standard taking experience from earlier versions into account. The GLUE schema has a *site entry* element, which describes the site identified, site location (longitude, latitude), site name and aggregated site resources. Some mandatory and several optional attributes such as site description,

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site location in a human readable format, administrator emails or site Web page were used in interoperation. Figure 1 indicates that all the mandatory attributes for a Grid site are provided by the GIN Top-level-BDII, which in turn may feed information into other Top-level-BDIIs (e.g. ARC) for the broadcast of interoperability information among the Grids.

Another fundamental challenge in the context of GIN-INFO is related to a general *lack of information*. Not all information systems publish all optional attributes, so a cross-Grid application implementation may encounter errors when it requires exactly that information. Of course these problems also arise if Grid sites do not publish this information correctly (e.g. not GLUE schema compliant).

It seems reasonable to consider that the above mentioned information could be useful in the context of service discovery of job execution endpoints (e.g. OGSA-BES [20] interface implementations) across Grid boundaries. Thus, missing or incorrect data could lead to problems when using this data in real use cases such as data staging between sites and simple job executions. In more detail, this leads to job submission errors with confusing error messages because the user sees an error from the job submission system; the native information system is correct, and the real error is in the translated information system. The pieces of information required have to be defined by the use cases and thus raise the demand to identify pieces of information required for cross-Grid use cases. In this context, the GLUE 2.0 working group is currently working on this particular issue.

The final approach uses the same set of attributes, but is slightly different to the initial architecture due to the administration overhead of providing a BDII for each Grid. Instead, Figure 2 illustrates that for each production Grid an information provider has been developed, re-using experience gained from the translators. In production scenarios, the information provider queries the corresponding Grid site and exposes the information in LDIF in accordance with the GLUE schema. In turn these information providers are used to provide the GIN Top-Level-BDII with information from all participating infrastructures using a generic provider in between. In turn this information lays the foundation for the ARC–BDII that is also a Top-Level-BDII, but publishing in accordance to the ARC schema. The ARC schema is used within the NDGF whose ARC middleware implements a scalable and dynamic distributed information system, which is capable of using this information for cross-Grid scenarios.

All in all, GIN-INFO provides components to fetch information out of nine production Grids that use different information services and schemas, namely APAC, DEISA, EGEE, NDGF, NGS, NAREGI, PRAGMA and TeraGrid. At the time of demonstrations, NAREGI uses the CIM schema, NDGF relies on the ARC schema and NGS uses the MDS2.4 schema of Globus Toolkit 2, and the rest use GLUE. When GLUE 2.0 becomes available and widely accepted, the use of different information schemas is hopefully obsolete.

The described interoperations were demonstrated at the Supercomputing 2006 and 2007 by using Google Earth showing information from all participating Grid sites. This demonstrated a common minimal set of attributes provided by various infrastructures and thus underlines that it is possible to interoperate in terms of information exchange. More information can be found in the GIN-INFO area of GIN on GridForge [1].

3.2. Data management and movement

In order to move and transfer data between production e-Science infrastructures, they must be interoperable using high-performance data transfers such as GridFTP [16] and data brokering

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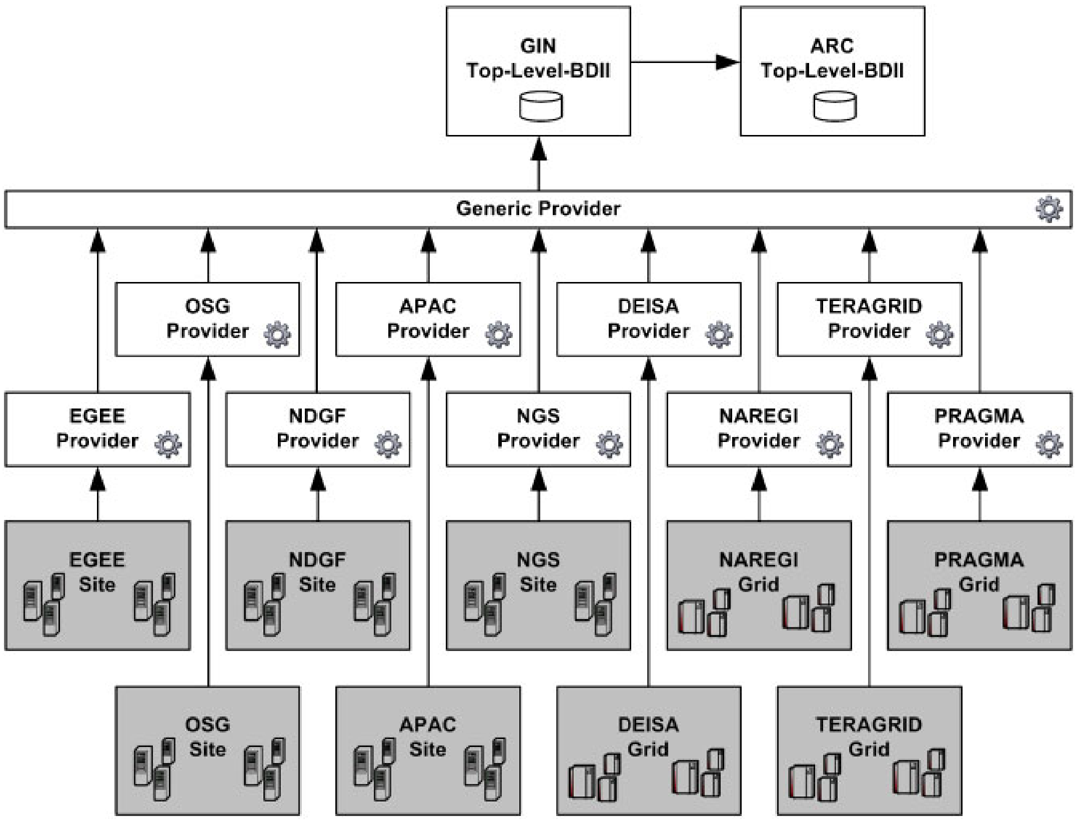

Figure 2. Information providers for different Grid systems.

technologies such as SRB [14] and SRM [15]. Therefore, the GIN-DATA area is working on interoperation of three different technologies. First, the GridFTP technology can be seen as the lowest common denominator for data movement in Grids today. Second, SRM as a standard asynchronous control interface to Grid storage systems; with more than six interoperating implementations, it is now an OGF standard achieved by the GSM-WG [25]. SRMs usually rely on GridFTP for data transfers. Finally, SRB implements a data Grid approach, a shared collection management system of multiple (distributed) storage systems that provides virtualization of whole shared data collections and their metadata. All these three mentioned technologies are widely deployed in production Grid infrastructures today.

Most production Grids use different implementations of the GridFTP protocols, but basic interoperation is typically achieved using test suites. Also, a subset of the GridFTP2 protocol is more and more implemented, for instance within dCache [26], Globus C and Java client libraries. At Supercomputing 2007, the NDGF demonstrated its production usage, which in turn lays the foundation for interoperation with any GridFTP2 compliant Grids. In addition, interoperation efforts on a pair-wise fashion for scientific scenarios are also undertaken world-wide. One example of such a scenario was demonstrated at Supercomputing 2007 showing interoperation between European DEISA and the Australian Grid in terms of data transfers using GridFTP. The fundamental goal of this scenario is to enable a cross-Grid scientific application job submission based on NAMD molecular dynamics suite [27] and to seamlessly work with the outcome afterwards. While the DEISA command line tool DESHL and its implied SAGA implementation was used for job submissions using JSDL, the file transfer between the Grids was successfully achieved by GridFTP implementations.

Besides these efforts for data movement, the efforts for data management are important as well and focus on access to storage via standard interfaces such as SRM. The GIN-DATA area achieved interoperations between different SRM implementations also using test suites, which focused on a core subset of the SRM specification. By using this subset nine production Grid sites were able to interoperate. While SRMs are based on a common interface specification, many advanced data management functions (e.g. space reservation) are optional. The error response when asking for a non-implemented feature is in most cases not clear enough to understand the real reason without contacting the administrator. Another challenge that the GIN-DATA group encountered was that the most SRM implementations within production Grids are tuned to use GridFTP as underlying data transfer protocol and thus run into problems when other protocols (e.g. HTTP) are being used in other production Grids.

The purpose of the SRM testing tool is to check compatibility and interoperability of SRMs according to the specification. Thus, the tool checks client-to-SRM adherence to the specification, as well as SRM-to-SRM remote copy capabilities. The basic tests include read access to a file in a remote Grid storage system managed by SRM. Furthermore, file replication for a registered user between two independent storage systems is tested. Finally, also space reservation and write access to a reserved space for a registered user in a remote Grid can be tested by the tool. To sum up, this tool helps to ensure production Grid interoperation between SRM implementations, and is being used by the SRM-collaborations.

Another GIN-DATA activity is to achieve SRB interoperation by establishing trust between different SRB-based data Grids. The SRB interoperation tests initially focused on single file replication and subsequently on replication of data collections between multiple federated Grid infrastructures. This included the federation of data Grids based on the SRB and replication of a collection into a federated data Grid. Another useful test is the use of remote procedures to extract provenance metadata and load the provenance metadata into a collection. Finally, tests have been done to test the use of extensible schema mechanisms to manage hierarchical metadata descriptions. To sum up, these tests were successfully run between 19 different Grid sites. The three most common problems found during these tests were the establishment of trust between the Grids that basically requires manual intervention today, interoperation between different versions of SRB and the identification of what metadata will be shared.

Finally, a more recent interoperation activity focused on data transfer between SRM and SRB in a scenario that uses advanced gLite data management tools. The trick is to use a GridFTP server developed for SRB, to endow it with an 'SRM information system' and to pretend it as the so-called classic storage element. This permits the gLite tools, both the File Transfer Service (FTS) and the so-called LCG-UTILS, to transfer files between SRMs and SRBs, with no development efforts required. This scenario is shown in Figure 3, which underlines that GridFTP and information systems are integral to SRM, and also shows how interoperation was achieved by having SRBs with a GridFTP layer on them and an added information system. In turn, higher-level Grid tools use data

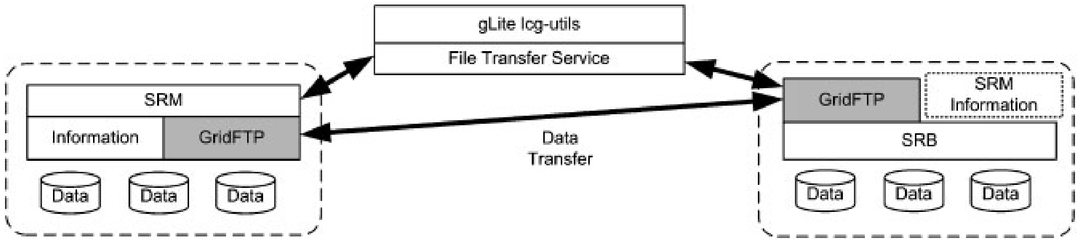

Figure 3. Access to SRB and SRM data via GridFTP in production Grid interoperations.

transport with GridFTP as the main entry point for SRB, whereas they use the SRM protocol with the SRMs. Traditionally, higher level tools like LCG-UTILS first make use of the information system for resource discovery and selection and with the developed interoperation, an end-user can access SRM and SRB data.

All of the GIN-DATA activities have been demonstrated at Supercomputing 2006 and 2007. Also, interoperation demonstrations in the context of the gLite AMGA Metadata Catalogue [28] have been shown. This technology is used in EGEE and provides access to relational databases. By using the OGF WS-DAIR specification [29], a standardized data access for different versions of gLite AMGA Metadata catalogue on different sites was achieved.

Finally, more information can be found in the GIN-DATA area of GIN on GridForge [1].

3.3. Job submission and management

There are a lot of production e-Science infrastructures that all support wide varieties of Grid middleware platforms and technologies that unfortunately provide *no commonly accepted interoperable interface for job submission and management*. For example, the gLite [30] middleware of EGEE uses the proprietary *Job Description Language* (JDL), Globus Toolkit's GRAM [31] of the TeraGrid accepts job descriptions in a proprietary *Resource Specification Language* (RSL) format and UNICORE 5 [32] of DEISA uses a proprietary job description named as *Abstract Job Objects* (AJO*s*). Hence, there is currently no standardized job description format in use within production Grids and no well-defined interface for job submission and management broadly adopted within e-Science infrastructures.

The lack of such a standard leads to rather complicated interoperation efforts using tweaks and workarounds. To provide an example, the EGEE-II project developed an interoperation between gLite and UNICORE using no standards at all. The objective of this interoperation scenario is to submit jobs from the EGEE infrastructure based on gLite to the DEISA infrastructure based on UNICORE 5. This interoperation is required as a fast short-term achievement by several e-Science initiatives such as the WISDOM project [33], which requires access to cycle farming resources in EGEE and massively parallel resources in DEISA.

Figure 4 shows this interoperation scenario that has been demonstrated at Supercomputing 2007. A scientist of the EGEE infrastructure uses a gLite User Interface (gLite UI) to submit the job that is intended to run on a computing resource managed by UNICORE. Like a job running on the EGEE infrastructure the user describes the job in a JDL file, but adds a special requirement for this

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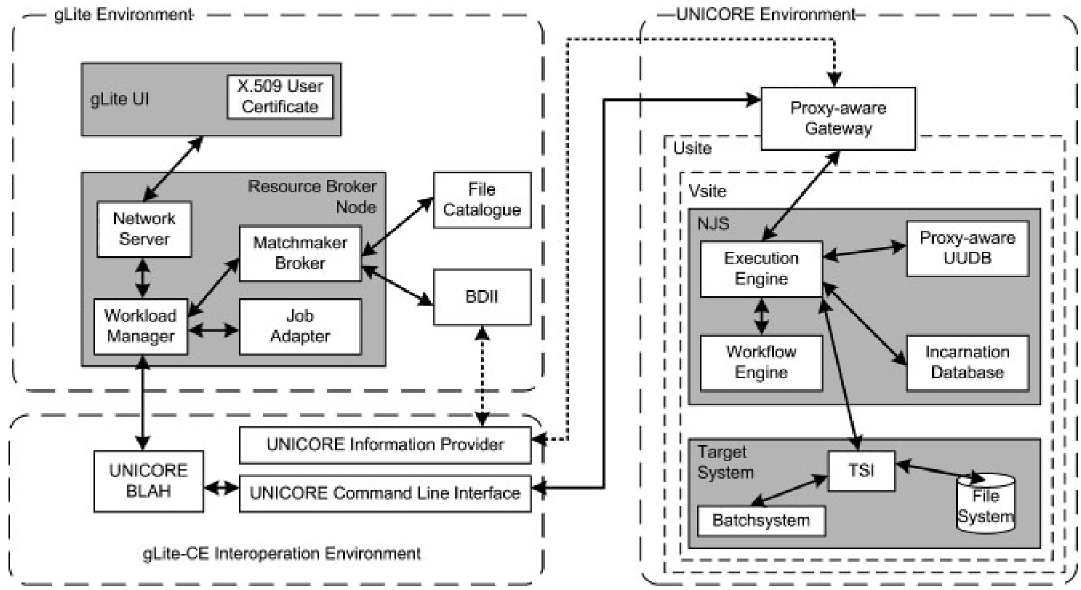

Figure 4. Interoperation of UNICORE 5 and gLite as short-term achievement.

job (i.e. other.GlueCEInfoLRMSType == 'UNICORE'). Through this requirement statement, the MatchMaker on the gLite Resource Broker (see Figure 4) is advised to choose a gLite Computing Element that is configured for transferring jobs to a UNICORE-based infrastructure, shown as gLite-CE Interoperation Environment in Figure 4. The gLite Resource Broker stores the so-called inputsandbox, i.e. the data transferred by the user from the gLite UI, and sends a job description including URIs of the input- and outputsandbox to the gLite-CE Interoperation Environment. If the user for example wants to execute a shell script, this script is send as part of the inputsandbox and stored on the gLite Resource Broker. When the job gets executed the inputsandbox is fetched by the compute resource, either a gLite Worker Node or a UNICORE Target System, for execution.

Also, in terms of security this interoperation scenario was a challenge since gLite relies on proxy certificates [34] while UNICORE only accepts full X.509 certificates. For the gLite Computing Element, Basic Local Ascii Helper (BLAH) scripts were implemented that allow for job submission to UNICORE and control of these jobs. The job submission script builds a UNICORE AJO based on the job description from the gLite Resource Broker. The AJO is signed and submitted using the users VOMS proxy certificate [35]. In the UNICORE environment the job arrives in the UNICORE Environment at the UNICORE Gateway (see Figure 4), which authenticates the so-called consignor of the job, i.e. the one who submitted the job. In order to accept job submissions consigned by proxy certificates, the UNICORE Gateway was modified as described in [36]. The UNICORE Network Job Supervisor (UNICORE NJS) uses the UNICORE User DataBase (UNICORE UUDB) to match the so-called endorser, i.e. the one who signed the job, to a UNIX userid on the Target system. In order to match proxy certificates to UNIX userids a new UUDB was implemented. This UUDB compares only parts of the certificates DN with the DataBase entry. If an entry was found, the job is forwarded to the Target System for execution. On the Target System, the users inputsandbox is fetched from the Resource Broker and the job is executed. Therefore, gLite Worker Node functionality, available for several systems, is needed on the Target System.

The example of the above mentioned interoperation scenario underlines the demand for a standard for job submission, including aligned security models. The OGSA-*Basic Execution Services* (OGSA-BES) [20] specification provides such an interface that accepts job descriptions in the standardized *Job Submission and Description Language* (JSDL) [37] format. The HPC-Basic Profile (BP) [38] combines both specifications together with some HPC-specific extensions to JSDL. Recently, many software providers have started to support the HPC-BP and thus many production Grids are evaluating the implementation of this interface in the corresponding middlewares. Therefore, the GIN-JOBS area also uses this interface to provide a proof-of-concept interoperation demonstration before this interface comes into production usage within real application scenarios.

It was commonly agreed within GIN that the use of HPC-BP makes more sense than providing yet another set of interoperable short-lived adapters for Globus GRAM, UNICORE or gLite environments. Also many commercial vendors (e.g. Platform Computing, Microsoft, IBM, Fujitsu, etc.) agreed to provide such an implementation of this interface for their technologies. They basically agreed because the JSDL specification is already standardized while the HPC extensions and the OGSA-BES specifications are mature enough to become OGF standards very soon.

Several interoperation efforts were demonstrated at the supercomputing 2006 and 2007 and particularly these demonstrations lead to interest in computer science media and news sections of online newspapers and reports, which in turn leads to high visibility for the standards. The GIN-JOBS group used *Transport Level Security* (TLS) [39] in combination with the WS-*Security Username Token Profile* [40] as the security mechanism. Even if this kind of security can be significantly improved, the interoperation was focusing on the interface level of OGSA-BES and the HPC-BP in order to be successful.

In this context, it is important that the OMII—Europe project [41] augment middleware—currently gLite, UNICORE and the Globus Toolkit—with OGSA-BES interfaces to lay the foundation for its adoption of this interface by middleware providers. Hence, this in turn lays the foundation for the usage of this interface and HPC-BP profile within production e-Science infrastructures in the near future. This will lead to at least three independent implementations of OGSA-BES; thus, the OGSA-BES specification and HPC-BP will change its status from proposed standard recommendation to full standard recommendation in OGF. In a later section, we will describe how the security setup in conjunction with an OGSA-BES interface can be significantly improved by using VOMS [42] during job submissions.

Closely related to job submission is also the tracking of resource usage and accounting, which is also highly required within e-Science infrastructures. At OGF19 and a follow-on meeting at CERN, we decided to stay basically with the GIN areas, but look on other important areas, and one of these areas is accounting. It lays the foundation for billing and pricing and thus may increase the uptake of Grids in the commercial scene and supports the sustainability of e-Science infrastructures by being not only dependent on funding of public bodies. Especially in interoperation scenarios accounting becomes a major challenge, not only by having different security setups and job submission technologies, but also due to the different nature of computing resources (farming vs HPC). These different computing resources consist of CPUs or, more recently, cores, which have a wide range of performance and thus makes it rather difficult to define valid pricing models for CPU/core usage.

At Supercomputing 2007, the OMII-Europe project participated in the GIN demonstrations with a showcase using the Distributed Grid Accounting System (DGAS) [43] and the Swedish Grid Accounting System (SGAS) [44]. DGAS is one of the accounting systems in gLite, while SGAS is not only the accounting system of SweGrid, but also, as a Globus Tech Preview, often used in Globus-based Grids. The goal of this scenario is to enable cross-Grid end-user usage records exchange between gLite-based and Globus-based Grids. These records are compliant with the OGF Usage Record Format (URF) [45] and consists of used CPUs, memory, job duration, just to list some recorded information. The records are exposed with the emerging OGF standard interface OGSA-Resource Usage Service (RUS) [21]. OMII-Europe augmented DGAS, SGAS and UNICORE 6 [46] with an OGSA-RUS interface to allow for cross-Grid usage record tracking and exchange. At Supercomputing 2007, interoperability between DGAS and SGAS was shown, and also OGSA-RUS-based monitoring solutions on top of UNICORE 6 have been shown by using the LLview application [47].

3.4. Cross-grid applications and operations

This section highlights several results of the interoperation efforts within the GIN-OPS area. It focuses on discovering issues, testing ideas and verifying solutions covering different aspects of Grid interoperation through running applications of scientific interest in the GIN testbed. This often presuppose interoperation in the other areas of GIN.

One example of interoperation demonstrated at the Supercomputing 2006 conference used the scientific program *Time-Dependent Density Functional Theory* (TDDFT) equation [48]. TDDFT is a molecular simulation method in computational quantum chemistry, and it treats multiple electrons excitation directly, using techniques from quantum mechanics. As a Grid application, TDDFT is built on Grid middleware Ninf-G. The efforts include interoperation in different scenarios, for instance between a run of the TDDFT application across the PRAGMA Grid, TeraGrid, OSG and NorduGrid. An interface between Ninf-G and NorduGrid had to be developed to enable interoperation to NorduGrid. In particular, this interoperation was achieved by running TDDFT on six heterogenous sites across these four Grids. In fact, it demonstrated that such a level of interoperation is neither automatic nor is it unattainable.

In addition to TDDFT jobs, the GIN-OPS group has also started a data-intensive application called the *Savannah fire simulation* in the GIN testbed to explore data-related interoperability issues. These experiments reveal a clear demand for job submission and management standards. Besides these issues the GIN-OPS group experiences revealed challenges in software support environments. Specifically, some Grids require site administrators to install a specific application (e.g. necessary libraries) and some Grids require applications to be self-contained (sandbox), which means that e-Scientists have to package all software that is needed. While the wider adoption of the sandbox method can be an option in interoperation, some Grids in the GIN-OPS group also worked on *community software areas* (CSA*s*) where users can install and share software. However, there could be difficulties in management and performance for some Grid environments, not to mention potential security problems. All in all, these experiments provided valuable lessons for Grid infrastructure supporters and Grid application users.

In this context it seems reasonable to mention the concept of virtual machines (VMs) as a software distribution and configuration method. The great advantage of VMs would be a more simple software configuration and deployment process that does not solve the interoperability in general but reduces the problem to that of VM hosting compatibility. However, this compatibility does not exist yet and recent studies reveal that the use of VMs in many production Grid environments, especially in HCP-driven environments such as DEISA or TeraGrid, significantly affect the performance of parallel applications. In addition, the middlewares deployed on these infrastructures have just started to support VM-based approaches, as in the case of the Globus Toolkit, while no VM support exists in UNICORE, gLite or ARC. As a consequence, the rather conservative deployment teams of production infrastructures have not yet found this technology mature enough to solve the application deployment problems, but observe their Grid adoption with great interest.

In addition to these efforts, the GIN-OPS group employed the SCMSWeb software [49], implemented cross-Grid resource testing and used to monitor sites by probing all GIN testbed resources periodically, provided near-realtime status of the authentication service, job submission and GridFTP of each GIN testbed site. Furthermore, GIN-OPS collaborated with members of GIN-INFO, implemented geographic mapping of GIN sites, and worked on a common schema to enable interoperation among various Grid monitoring software.

Another area of cross-Grid applications is related to the GIN *resource testing portal* that provides access to the various GIN VO resources and monitors their availability. The portal provides two services: first, it runs a monitoring service to check resources of the GIN VO; second, it offers a workflow editor and engine to create and run workflows on resources. These services are built on Grid Execution Management for Legacy Code Applications (GEMLCA) [50], Grid Monitoring Tool (GMT) [51] and the P-GRADE portal [52].

The p-grade portal [53] is a workflow-oriented portal and application hosting environment based on GridSphere. The portal is able to manage Grid certificates, to define Grid environments, to create and modify workflow applications, to control the execution of workflow applications on Grid resources and to monitor and visualize the progress of workflows and their jobs. GEMLCA supports the deployment of legacy applications as Grid services without re-engineering their codes. GEMCLA was integrated with the P-GRADE Grid portal to provide a user-friendly interface to deploy, execute and retrieve results from legacy applications. To access both resource- and service-oriented Grids, GEMCLA was extended by the GEMCLA Repository (GEMCLA-R). GEMCLA-R enables the legacy code owner to publish the application in the repository and allow authorized users to use the legacy code. GEMCLA-R submits the legacy code as a job to GT2- and gLite-based production Grids.

In terms of monitoring Grid resources of the GIN VO, a monitoring service is offered by GMT that uses MDS4 [19] to collect, store and index information about resources and control resource monitoring. GMT incorporates a set of probes to monitor basic network communication and Globus toolkit functionality, local job managers and GEMCLA services. GMT was integrated as a portlet with the P-GRADE portal. The portlet queries the MDS4 to retrieve the probes' results and present them. System administrators can configure the MDS4 service to run the probes at different pre-defined intervals. Currently, GMT runs 44 probes on GIN VO resources representing the EGEE Grid, NGS, OSG and TeraGrid. A snapshot of the P-GRADE portal is shown in Figure 5 showing how GT2 and LCG-based Grids are connected in one user-friendly GUI.

In terms of running applications on multiple Grids, the Resource Testing Portal supports workflow-level interoperation among resource- and service-oriented Grids. At Supercomputing 2006 and 2007,

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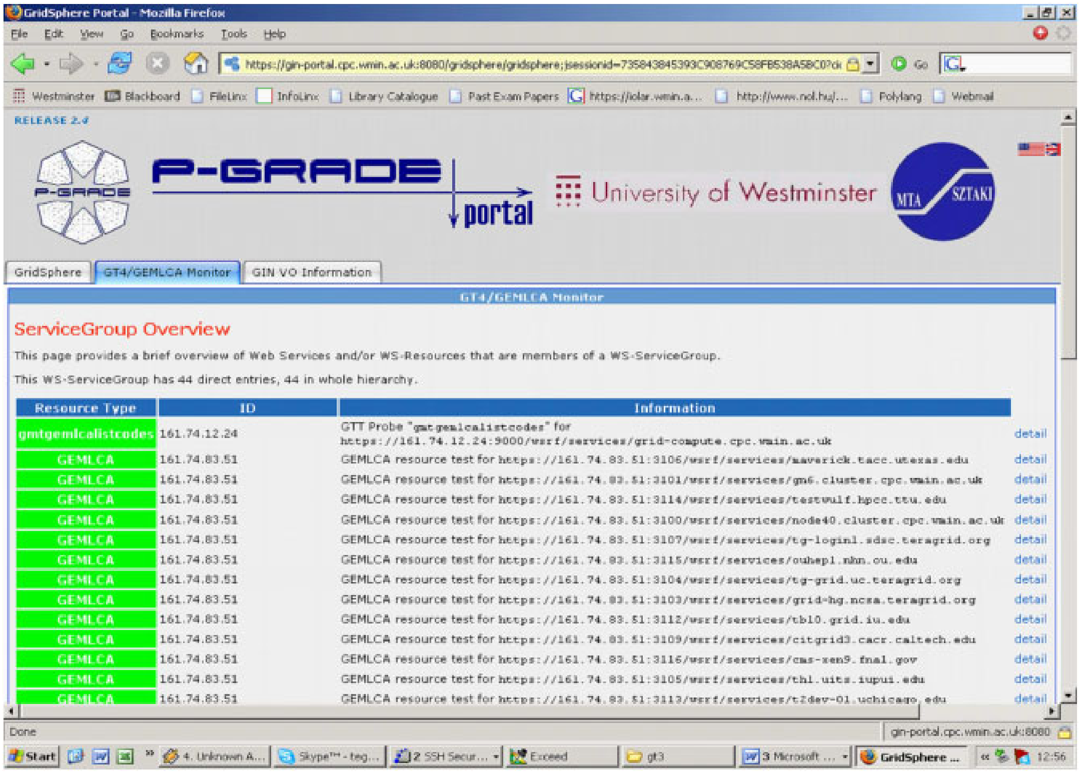

Figure 5. Connecting GT2 and LCG-based Grids accessible via portals.

GIN-OPS demonstrated how to run jobs on Grids with their resources accessing the EGEE Grid, NGS, OSG and TG using the CHARMM application. All in all, the Resource Testing Portal supports access to multiple Grids, for example LCG- and Globus-based Grids. The portal connects these Grids and maps the execution of different workflow components to different resources in different Grids. As the portal is also integrated with GEMLCA-R, users can browse it and select and run executables published by other users.

Another example out of the application area is a bit close to long lasting production efforts. These application efforts have been conducted in collaboration with the OMII-Europe project [41]. This project deals with interoperability in key areas such as job submission, accounting, VO management, database access and portals. In more detail, the project augments the Grid middleware systems UNICORE, gLite, Globus Toolkits and CROWN with certain standards such as OGSA-BES, JSDL, HPC-BP, UR, OGSA-RUS, just to list some. Also, it makes these middleware systems interoperable with technologies such as OGSA-DAI and GridSphere. OMII-Europe is one of the key contributors to the GIN efforts and works on scientific use cases such as the WISDOM project.

In more detail, the WISDOM project is a project that aims to significantly reduce the time and costs in drug development by using in silico drug discovery techniques. Technically speaking, the overall scientific workflow can be splitted into two parts as described in Riedel et al. [54]. The first part

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uses the EGEE infrastructure for large in silico docking, which is a computational method for the prediction of whether one molecule will bind to another. This part uses cycle farming resources in EGEE in terms of high throughput computing (HTC). This means that the single jobs do not interact with each other and are thus referred to as embarrassingly parallel. Applications that are used in this part of the workflow are AutoDock and FlexX that are both provided on the EGEE infrastructure. The output of this first part computed on EGEE is a list of the best chemical compounds that might be potential drugs and thus not the final solution.

Therefore, the second part of the scientific workflow is concerned with the refinement of the best compound list using molecular dynamics (MD) techniques. For this part, the scientists have started to use massively parallel resources in DEISA using the highly scalable AMBER MD package. All in all, the goal of this interoperability application is to accelerate drug discovery using EGEE and DEISA together. In fact, this application can be seen as an example for a whole class of interoperability applications that require access to both HTC and HPC resources.

3.5. Authorization and identity management

A functional authentication and authorization system is foundational to most of the other interoperation activities within e-Science infrastructures. The base use case is identity-based authorization at the service level with any further authorization restrictions enforced inside the service at the base internal system level. More advanced use cases include setting Grid permissions for members of specific groups or for end-users with a certain role within a VO.

These services are typically provided by a *Virtual Organization Membership Service* (VOMS), so GIN-AUTH provides a GIN VOMS service to permit interoperation testing without compromising security in production VOMS servers. VOMS is widely adopted in production Grids today and the two basic services that are provided by VOMS are the management of a list of members of a VO and signing attribute statements attesting to the subject's group/project membership or roles.

The creation of the GIN VO for testing purposes containing a limited number of staff from the participating Grids introduced another point of confusion for end-users of the system. Frequently, it was misunderstood that membership in the GIN VO was the method by which one gained access to resources from participating Grids to establish cross-Grid application interoperation—staff actually have access to their own Grids using their own Grid's VO, but no access to other Grids. This was a persistent problem because part of the GIN baseline activity was a standard series of application tests to establish functional interoperation. This was also a problem, because the GIN VO had pre-negotiated access to all the participating Grids, a step that was viewed as a significant barrier to e-Science VOs wishing to get started with multi-Grid interoperations.

Therefore, the GIN-AUTH group developed an Acceptable Use Policy (AUP) for VO membership. The AUP for the GIN VO can serve as a model for other VOs wishing to establish serious multi-Grid interoperations. It was agreed among the participating Grids that this AUP met most of their requirements and established a good baseline for VOs wishing to register with new Grids. There may be additional requirements for individual Grid or e-Science infrastructures, but those are typically few and deal with Grid-specific policies and procedures. The AUP is publicly available at [1] for use in e-Science infrastructures that would like to engage in interoperation scenarios.

More recently, the GIN VO is registered in OSG as operational VO today, because members of PRAGMA require access on Fermilab resources of OSG. This underlines the real-world recognition of the GIN efforts and its influence in world-wide production Grids. The scientific scenario is a biology PRAGMA application within the GIN VO that is ready to be run on OSG resources using the Nimrod/G Grid parametric modeling and middleware tool.

More challenges occur during the accreditation of CAs currently in use within e-Science infrastructures. Several of the Grids have internal processes for vetting CAs from whom they will accept credentials and there was no universal system for selecting or ranking a common set of CAs. Therefore, the GIN-AUTH team took the decision to concentrate on the *International Grid Trust Federation* (IGTF) [55] set of regional *Policy Management Authorities* (PMAs) list of accredited CAs. These represent a common set of recognized identity providers. While this decision allowed us to clearly identify a common set of mutually acceptable identity sources and a process for accrediting new ones, a few residual problems were uncovered.

Despite the agreement on credentials from IGTF sources being the commonly accepted set of credentials, end-users frequently made the presumption that because Grids X and Y are participating in GIN, that any credential that worked with Grid X would also work for communicating with Grid Y. Since there remain several Grids that recognize local or lower assurance CAs for internal purposes, this presumption is incorrect and leads to much confusion and frustration in end-users getting started with interoperation between Grids. It is particularly difficult for end-users to recognize beforehand when dealing with service credentials issued by a local CA (non-IGTF). GIN-AUTH strongly recommended and encouraged e-Science infrastructure administrators that any service for multi-Grid interoperation uses only credentials issued by an IGTF accredited source to avoid such problems in the next years.

Another important work of the GIN-AUTH group is related to the OGSA-BES adoption and the HPC-BP profile. As mentioned above, the definition of these interfaces and profiles are a first good step toward the right direction; however, from the GIN perspective, both can be significantly improved. While a plain OGSA-BES discussion is given later in the text, we here outline a more advanced security setup that is needed in real production Grids taking the requirement of an Attribute Authority (AA) [56] like VOMS (or Shibboleth) into account.

In fact, the OMII-Europe project demonstrated at Supercomputing 2007 a scenario using OGSA-BES services and a VOMS based on the Security Assertion Markup Language (SAML) [57] as shown in Figure 6. The scenario shown has the potential to provide the long-term interoperability between UNICORE 6 and gLite as requested by several scientific projects such as WISDOM. Hence, it is an evolution of the interoperation between UNICORE 5 and gLite described in the context of job management when DEISA and EGEE have adopted these new developments. The SAML-based AA

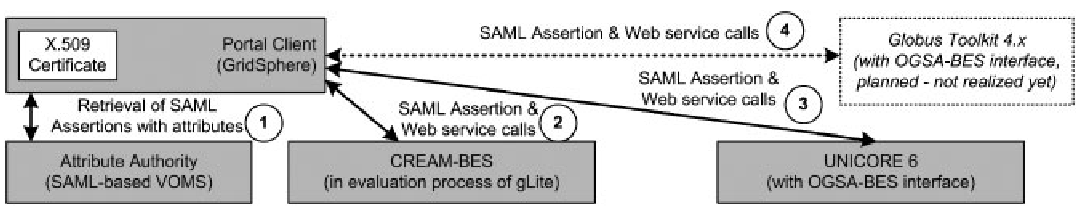

Figure 6. SAML-based Attribute Authority (here VOMS) as crucial authorization element releasing SAML assertions with attribute information used in cross-Grid authorization. SAML assertions can be transported with Web service invocations for later authorization checks within the middlewares.

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releases signed SAML assertions [57] that consist of attributes with information about group/project membership or roles of end-users. These SAML assertions are then used in conjunction with Web service invocations (e.g. an OGSA-BES call) and the Grid middleware (trusting the AA) is using these SAML assertions for authorization checks (e.g. using XACML-based policies [58]).

SAML-based scenarios could become generally accepted since SAML is already used in industry, including SAML delegation. This approach is discussed with the OGSA-AuthZ group to start a GIN spin-off activity in collaboration with security experts to work on an advanced security profile for OGF Web services interface standards. In fact, one GIN session in OGF23 in Barcelona was held for the discussion of security problems in interoperability.

4. LESSONS LEARNED

The fundamental goals of GIN are gaining experience in world-wide interoperation scenarios and providing feedback to standardization groups of OGF. In this chapter we take lessons learned from the last years into account, including experiences from Supercomputing 2006 and 2007 demonstrations as well as numerous OGF sessions and interoperation experiments in the field. In the later conclusions, on the other hand, we focus more on the concrete groups and their results and recommendations instead of general GIN infrastructure views presented in the following sections.

4.1. SW providers meet GIN and standards

At OGF21, GIN organized a session bringing SW providers and OGF standardization groups together with the GIN infrastructures. The idea was to have a round table (not exactly a panel) to discuss current issues in standards and to identify what are promising standards in the near to mid-term future. Participants in the session represented Grid Middleware technologies such as Globus Toolkit and UNICORE, and middleware enhancers such as gLite, ARC, GRIA, GridWay, CROWN, OMII-UK and OMII-Europe. Also members of well-known Grid software stacks participated such as SRB/iRODS and Condor. Of course, most GIN infrastructures have been present in the session.

Initial discussions focused on information schemas and it was generally agreed among all that GLUE 2.0 is a promising emerging standard that the middleware providers will follow and also the infrastructures would deploy. Part of the discussion were issues stated from business about sensitive elements within the GLUE 2.0 schema, which should not be exposed, but during the discussion it turns out that GLUE as a basic schema is a perfect base for later dynamic aggregation of information (even business contents) exposed on a trusted per-domain base. In addition, discussions with GLUE people and data software providers (OGSA-DAI, SRB) led to the demand of describing data resources/services with GLUE as well.

Other discussions have been around the wide variety of security setups and standards in the field. There are systems using proxies while others use full X.509 certificates, systems using classic VOMS (i.e. VOMS Proxies) and others using the SAML-based VOMS and many other differences leading to big obstacles in interoperability testings. Generally it was agreed that there are enough standards out there, but they have been brought together as a profile usable within infrastructures. Another issue raised was that some groups in OGF release security standards (i.e. Express AuthN profile) bypassing any security group of OGF. This potentially leads to inconsistency in security roadmaps for the broader Grid community and also narrows the scope of only using a subset of security standards available and known by security experts. As a conclusion of this discussion, GIN and the OGSA-AuthZ group jointly started a security interoperability spin-off activity. As a first result, GIN organized a session at OGF23 trying to work on a more advanced security profile usable in GIN infrastructures since demonstrated results (e.g. with Username/Password) would not be deployed on infrastructures and are just for interoperability testings. Topics discussed in this session have been authorization/authentication in general, restricted delegation and third-party credential forwarding in particular.

Discussions in the context of computational resource access lead to general agreement that OGSA-BES is not enough for production usage, but a good first step in the right direction. There are issues from all major Grid middleware providers such as Globus, UNICORE, gLite (CREAM-BES), ARC, CROWN and numerous others. The issues lead to the fact that the most implement extensions to OGSA-BES, which in turn makes the interface implementations not interoperable although the core interface is the same. For instance, the state model currently used will require extension from many developers of the simple OGSA-BES model (Pending/Running/Failed/Finished/Terminated). Hence, extension will follow the ‘state specialization’ instructions and by doing so, other Grid clients cannot interpret the status specialized for one technology. For instance, there is one ARC state difficult to map to the OGSA-BES model: Jobs that are not available any longer on the computing service but were served some time ago (within a grace period) enter into the ‘DELETED’ state. Also, the UNICORE state model (i.e. explicit start of activity required) is quite different from the OGSA-BES model.

There are many other limitations such as the lack of explicit operations to cleanup end-user space and old activities, the demand for a meta-BES-Factory that creates the BES-Factory as a stateful service in the context of the optional WS-RF specification support and the demand for better integration of secure data staging technologies, but most notable better security setups are aligned with OGSA-BES. There is never the vanilla OGSA-BES interface deployed in the infrastructures; it is always aligned with a well-defined security setup (e.g. using attribute-based authorization). The initially adopted Username Token Profile is not realistic for GIN infrastructures. Hence, due to the many issues on such an important interface, the GIN group decided to start a spin-off activity and pursue the problems with OGSA-BES and to provide feedback to the group so that version 2.0 might be better suited for production usage.

Another major discussion topic was the storage and data access, including movement of data between different infrastructures. Although GIN did some workarounds, it is still a major challenge to do this in a production scenario. Some rely on SRMs, some on SRBs, others use just GridFTP, while some will not open a port range for GridFTP. Even getting two SRM implementations to work together is not straightforward. Also, the data management systems work on customized features (i.e. iRods and preservation environments) that are not covered by a standard SRM interface, but in use by end-users during production scenarios. One conclusion that can be drawn from the discussion is the requirement for another higher-level data movement interface that might be the OGSA-Data Movement Interface (OGSA-DMI) [59]. However, it was also stated that this interface still needs time to evolve and had not focused so far on the real complicated things (e.g. third party credential forwarding).

To sum up, fundamental lessons learned from this session are that many standards are still not improved/stable enough to be deployed on GIN infrastructures, although there is already work

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going into the right directions (i.e. OGSA-BES, OGSA-DMI). Another conclusion is that we urgently require better security profiles, advanced profiles that cover realistic use cases (e.g. using attribute authorities such as VOMS or Shibboleth). There are many security specifications out there; the question is how you align them in several profiles. Both lessons learned lead to GIN spin-off activities that are now actively pursued. The result will be presented in future OGFs and fed into the standardization process of the respective groups.

4.2. Standard adoptions

A crucial point within GIN is the adoption of OGF (and other) standards. The rather slow process of OGF specification standardization leads to a slow adoption of standards by the middleware providers. This in turn leads to the fact that many infrastructure had to create their own solutions in the past while emerging standards have been developed slowly in parallel. When the standard is available, the question is why an infrastructure should change their well-tested technologies to systems that have just been developed and not very well tested.

In addition, the standards themselves seem to change itself rather often (i.e. change from OGSI as base technology to WS-RF and WS-I in the past). This became even more crucial looking at the adoption times and deployment roll-out schedules of GIN infrastructures. A roll-out of a certain new technology really takes time and is often not even user-friendly (e.g. change of client technologies for end-users). The question arises if interoperation in a pair-wise fashion for dedicated scenarios is more realistic sometimes.

Therefore, at OGF22 we had a session in the specification adoption track to get an overview of which standards are adopted (and planned) in which infrastructures in the near to mid-term future. We have summarized the result in Table II, which basically lists the standard adoptions of the middleware systems deployed on the infrastructures.

Table II. Standard adoptions of Grid Middleware deployed on GIN Infrastructures.

	gLite	Globus Toolkit	UNICORE	ARC	NAREGI	NGS
Security	X.509 VOMS SAML XACML	X.509 VOMS SAML XACML	X.509 VOMS SAML XACML	X.509 VOMS SAML XACML	X.509 VOMS SAML XACML	X.509 VOMS
Information Systems	GLUE XML	GLUE XML	GLUE2 XML	GLUE2 XML	CIM SQL	GLUE XML
Accounting	RUS/UR		RUS/UR	RUS/UR	RUS/UR	RUS/UR
Job Management	BES JSDL DRMAA	BES JSDL DRMAA	BES JSDL DRMAA	BES JSDL DRMAA	JSDL	BES JSDL
Data Management	GridFTP SRM2.2	GridFTP DAIS	ByteIO	GridFTP SRM2.2	GridFTP GFS	GridFTP DAIS

4.3. Conclusions drawn from the lessons learned

We draw first conclusions from Table II, which shows where similarities and differences exist in terms of standardization adoptions that are relevant to GIN infrastructures. In fact, we observe an emerging dominance of the standards X.509, SAML, XACML, OGSA-BES, JSDL, OGSA-RUS and UR. In addition, the concept of VOMS to perform attribute-based authorization is also established in the listed GIN infrastructures. Hence, the standardization efforts in the context of security, accounting, and job management are quite far and thus already relevant for the GIN infrastructures.

On the other hand, we observe that many technologies of GIN infrastructures follow different information schemas although the GLUE work is dominant, but unfortunately still relies on different versions of GLUE. In this context, the harmonization work that is being carried out by OGF becomes important, especially in the context of GLUE and CIM and thus between OGF and DMTF. Different content schemas are critical and thus it is important that the recent efforts around GLUE2 and outreach to DMTF are performed by OGF.

We also observe that the data management area seems not to have an emerging dominant practice. While most technologies use GridFTP, others rely on ByteIO or adapt the WS-DAID specification implementation. This has several reasons. First, some GIN production infrastructures rely on distributed parallel file systems, like for instance, the General Parallel File System (GPFS) within DEISA, and thus data transfer support with GridFTP within OGSA-BES was no major requirement in the past. On the contrary, the SRM specification of OGF evolved among certain production Grids (i.e. EGEE and NDGF) that both were clearly driven by the needs of the Large Hadron Collider (LHC). As a consequence, gLite and ARC support the use of SRM interface implementations. Other technologies such as Globus Toolkits have been driven by the needs to support relational databases in Grid environments and thus WS-DAID support exists.

Second, we can conclude that data management is typically considered to be second priority behind job submission and its related technologies (i.e. security, accounting) in order to support the basic Grid usage scenarios. As a consequence, the efforts of standardization and joint usage have been less than with job submission technologies. However, we observe that more recently standardization efforts of OGF (i.e. SRM) attract the wider Grid community and thus we expect broader adoption in the near to mid-term future.

These conclusions basically point the way to where further best practices and standardization efforts need to be concentrated. Therefore, although this paper provides general conclusions at the end, we provide here a list of the major best practices and standardization efforts that should be undertaken as identified by all GIN efforts.

- Open standards have to evolve more quickly taking the requirements from production Grids (and their end-users) into account. Hence, there should never be a specification defined by OGF that is not aligned with a real implementation that is considered to be deployed on production Grids (or equivalent in industrial/commercial Grids). Hence, not only the technology providers should be in the loop, but also deployment teams of the infrastructures that state that the standard implementation can be realisticaly deployed. To provide an example, we observed that the first implementation of the WS-DAIS standard was not usable and raised serious concerns from end-users. The same is valid for early OGSA-RUS specification implementations.
- The devil is in the details. There are still areas of standardization that are considered to be non-important, e.g. the mentioned worker node profile. However, we observe that even

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small non-standardized solutions could break the whole interoperation/interoperability. To provide an example, computational jobs that require certain environment variables for several application functionality/options simply fail when they are submitted through different OGSA-BES compliant interfaces although using JSDL. Thus, standardization efforts should be in general more detailed, and if not possible, at least providing profiles for these kind of details.

- We observed that data management in general still needs standardization efforts (and attention). To provide an example, the functionality of a service that provides logical file name mappings to physical file name mappings is required in many production Grid infrastructures. But many of them use different technologies for this (AMGA Metadata Catalog, LFC of gLite, etc.). In addition, although the SRM interface specification is a good step forward, we raise a demand for a higher-level interface that may be provided in the near future via the OGSA-DMI specification and related efforts.
- Some standards have to be continuously improved to take new requirements into account. To provide an example, JSDL is one of the most adopted standards of OGF; however, we observed that many required parts of JSDL are extensions (i.e. SPMD) or do not cover recent requirements like the specification of network topologies when submitting computational jobs to recent hardware architectures (i.e. BlueGene systems).
- Another area where important standardization work is missing are the links between certain specifications. Adopting one specification is typically easy but this does not mean that the most use cases run with the implementation since there is often a close coupling with another specification. To provide an example, OGSA-BES implementations are clearly the technologies to submit computational jobs, while their data staging JSDL elements raise a demand to exactly specify the link to data management specifications such as SRM, WS-DAIS, GridFTP, ByteIO. Hence, even if systems have adopted OGSA-BES, the missing link to data management breaks jobs that require data staging. The recent OGF activities of the HPC File Staging Profile (FSP) [60] or OGSA-DMI are a first step toward the right direction, but clearly not enough for GIN production infrastructures.
- Security is often out of scope and often mentioned briefly in a specification. But the truth is that security is often not only the most important part in infrastructure interoperability in rather general parts (i.e. transport level), but also in particular parts (i.e. credential delegation for third-party transfers) and thus affect the specification directly. In other words, security is typically orthogonal to a functional specification like OGSA-BES and thus there should be more standardization work on how these standards can be used with adopted security specifications such as SAML or XACML. In this context, it is obvious that the used security standards often differ from commercial providers and academic providers that again raise the requirement for more profiling in this area.

5. RELATED WORK

There are many pair-wise efforts in the field of interoperation and interoperability within e-Science communities and Grid projects. These efforts typically include the interoperation between one specific version of a technology with another one.

EGEE and OSG have a long ongoing pairwise interoperation effort and have achieved full interoperability that is now moved into a sustainable model. Experiences of this work were fed back into GIN and in particular bootstrapped the work on GIN-INFO. Similar efforts are ongoing between EGEE and NAREGI, EGEE and NorduGrid, OSG and TeraGrid, OSG and PRAGMA. In addition, middleware interoperability efforts are also ongoing between gLite (EGEE) and UNICORE (DEISA) as well as gLite (EGEE) and ARC (NorduGrid) as part of the EGEE-II project.

To provide an example, one of the major activities in reaching interoperation between two production Grids is conducted within the EGEE-II project: a particular activity within this project focuses on the interoperation between specific versions of gLite and UNICORE. Specifically, interoperation uses the non-Web services-based gLite middleware of EGEE with the non-Web services-based production UNICORE 5 of DEISA. The fundamental goal of this activity is to work on job submission mechanisms to enable interoperation between EGEE (HEP and other scientific communities) and DEISA (HPC community) on a technical level. A closer look reveals that this interoperation is not based on open standards and is fundamentally based on VOMS. Although related work, members of this activity participated in GIN and demonstrated their results at the Supercomputing 2007.

The EchoGrid project [61] performs so-called Grid Plugtest. The objectives of these tests is to improve interoperability mechanisms of Grid middleware, and to learn, through user experiences, deployments and open discussions, about the current status of Grid infrastructures used in Europe and China. This also includes Grid middleware that is in use on each side as well as future features and interoperability mechanisms needed for the Grid.

Another interesting related work is the EU-IndiaGrid, which seeks to achieve interoperability between the European infrastructures (EGEE and DEISA) and the Globus-based GARUDA [62]. GARUDA is the national Grid of India currently evolving to a full production Grid. The project develops an architecture that allows for seamless cross-Grid usage so that e-Scientists of India and Europe can work together to achieve their goals. One particular example application is related to quantum atomistic simulation using the different scales of systems available in GARUDA, EGEE and DEISA. There is also the EU-ChinaGrid project, which seeks to develop interoperability between the European infrastructure EGEE and CNGRID [63].

Related work in authorization and authentication is undertaken by the German IVOM project [64], which focuses on the interoperability of VO management technologies in the German national Grid D-Grid [4]. This is especially interesting since D-Grid is running Globus Toolkits, gLite and UNICORE. Members of IVOM have started to work in GIN.

Finally, there are certainly many other projects dealing with interoperability (e.g. EU-MedGrid interoperability with the Tunisian national Grid GTRS [65] or BRIDGE [66]) that are all invited to participate within GIN in the future.

6. CONCLUSIONS

This paper describes the results of the GIN-CG until early 2008, mentioning the highlights of interoperation demonstrations at the Supercomputing 2006 and 2007 conference, and numerous OGF sessions. These initial demonstrations provided massive insights into the process of enabling interoperation among production Grids and e-Science infrastructures in all the different areas of GIN.

Within GIN-INFO, all information systems are rather similar in their scope and partly also in their functionality. Therefore, the usage and development of information providers to populate systems was easier than expected and can be recommended for production Grids today. This was in particular the case, because the query mechanisms to extract the data were often based on LDAP, basic WS calls or open standards such as WS-RF. To sum up, querying an information system and populating another was rather straightforward. More difficult challenges were revealed in the output of queries, where information is expected to conform to a dedicated schema. In general, the Grid community can live with different information systems but not with different content schemas (e.g. GLUE or CIM). If there is a use case that needs to be done across all Grid infrastructures, then the information we need for these use cases must be present and in agreement. Also motivated by the efforts undertaken within GIN, the newly formed GLUE-WG of the OGF works toward a general content schema acceptable by the broader Grid community.

To demonstrate the feasibility of the interoperation of different information systems and schemas, the GIN-INFO area demonstrated the Grid site on a world map use case. Hence, the GIN-INFO area has successfully shown that Grids can be interoperable with respect to information sharing and exchange, because the GIN Top-Level BDII contains information about all participating production Grid infrastructures.

The GIN-JOBS area demonstrated that production Grids are able to use upcoming standardized interfaces for cross-Grid job submission and management. This was particularly achieved by using the HPC-BP and the emerging standards OGSA-BES and JSDL. Hence, typically it makes no sense to work on adapters or hacks between the different job submission technologies when a reasonable technology is soon to be standardized. However, we also have shown that some scenarios require fast short-term solutions such as in the case of the WISDOM project that requires interoperation between EGEE and DEISA as soon as possible. At the time of writing, the HPC-BP and OGSA-BES specifications as well as the HPC extensions of JSDL are released as OGF recommendations and will soon become an official OGF proposed recommendation. This will lead to even more adoption by middleware providers and thus a wider use of these interfaces within production e-Science infrastructures in the near future. In fact, also the cross-Grid operations from GIN-OPS revealed that such a standardized interface is a necessary requirement for production e-Science infrastructures, especially when dealing with grand challenges (e.g. protein folding or global weather prediction) in interoperation scenarios. In these scenarios, the use of portals such as the P-Grade resource portal becomes more and more useful instead of fat middleware clients.

The efforts of the GIN-DATA group have shown that interoperation between different Grid and e-Science infrastructures can be established via GridFTP, SRB and various SRM implementations, and in fact all three components can be brought to work together. However, it is not a straightforward task. Apart from improvements in information about the service configurations (e.g. supported versions, location of storage areas, etc.), the main issues for productive interoperation are in the areas of network tuning (e.g. advanced reserved dedicated network connections) and firewall management.

The GIN-AUTH group has shown that the base functionality of an identity-based authentication and authorization system is in place. There is a working federation of the current major Grid credential generators (the IGTF) and production Grid infrastructures that can form the basis of a global interoperation infrastructure. Also we have shown that the GIN group has transformed into a platform to ease collaboration between researchers and resource owners across the globe by the fact that real production Grids are taking the GIN VO seriously and integrating them into their access control systems as valid VO. The GIN VO is now an officially registered VO in OSG to access Fermilab resources in OSG by members of PRAGMA. Hopefully, other world-wide Grid infrastructure will think similar if they would like to interoperate with other Grid and e-Science infrastructures.

In order to have a strong link into research topics about interoperation and interoperability, the GIN group organized (together with OMII-Europe) the first International Grid Interoperation and Interoperability Workshop (IGIIW) at the e-Science 2007 conference in Bangalore. The method of interoperation and interoperability by gaining access to a wide variety of resources becomes more and more the interest of the Grid community and thus the workshop has been used to link different communities and create new cross-Grid collaborations. This workshop was also beneficial to understand still major open issues in interoperations today and provided additional topics for the further roadmap of the GIN group. In fact, GIN also prepared a second IGIIW workshop at the e-Science 2008.

Technically, the described interoperation components can be used today by e-Scientists within these infrastructures even if there is a negotiation phase needed to agree on resource usage with the production e-Science infrastructures. In collaboration with the recently started project OGF-Europe especially such negotiation questions might be solved in the future by setting up policies that ease the cross-Grid usage at the policy-level. At the technical level, the GIN efforts and the Supercomputing demonstrations provided a good first start toward world-wide interoperable e-Science infrastructures and emphasize that common open standards as defined by OGF, DMTF, IETF, W3C or OASIS are absolutely needed.

Finally, it is important to mention that the funding to support Grid and e-Science infrastructure-related topics is decreasing. This will have a major impact in potential scientific breakthroughs that will not be happening due to decreasing support and manpower in Grids. In fact, we know that the funding in U.S. was significantly decreased for Grid-related topics. Thus, most of the GIN demonstration efforts have been supported by European funding agencies, which also decrease the amount of money available for Grid-related research, e.g. by the discontinuation of OMII-Europe while this project was significantly contributing to OGF in general and GIN in particular. To sum up, the decrease of available funding could lead to serious sustainability problems for infrastructures and will certainly decrease the efforts for cross-Grid usage models that are typically based on a best efforts basis.

In this sense, it is important that the world-wide operating Grid and e-Science infrastructures work more closer together instead of working against each other, for instance by contributing to the GIN activity. This is particularly important since other communities such as the HPC community are well established over the years and thus Grid, as a rather new concept, has to first prove its broader usefulness. In the past, world-wide Grids have been focused on computational Grids instead of realizing the real Grid vision, which integrates all kinds of Grid resources far beyond the scope of computational resources (e.g. telescopes, colliders, or other large-scale instruments). Therefore, the recent evolution of the many-core and multi-core systems in HPC and the Amazon's Elastic Computing Cloud (EC2) [67] concept have led to serious considerations if the Grid concept will remain, even if these systems or concepts only provide computational- (and data) related technologies.

To conclude, only if all infrastructures follow the GIN approach of a *United Federation of Infrastructures* including national e-Science infrastructures as well as international ones, we are able to support the uptake of Grids in the future, which in turn provides funding to sustain our daily-used infrastructures to achieve scientific breakthroughs in e-Science.

Glossary

AA	Attribute Authority
AJO	Abstract Job Object
AMBER	Assisted Model Building with Energy Refinement
AMGA	ARDA Metadata Grid Application
APAC	Australian Partnership for Advanced Computing
ARC	Advanced Resource Connector
AUP	Acceptable Use Policy
AUTHN	Authentication
AUTHZ	Authorization
BDII	Berkeley Database Information Index
BLAH	Basic Local ASCII Helper
CA	Certificate Authority
CE	Computing Element
CHARMM	Chemistry at HARvard Molecular Mechanics
CIM	Common Information Model
CSA	Community Software Areas
DGAS	Distributed Grid Accounting System
DMTF	Distributed Management Task Force
DN	Distinguished Name
DEISA	Distributed European Infrastructure for Supercomputing Applications
DESHL	DEISA Shell
DRMAA	Distributed Resource Management Allocation API
EC2	Amazon's Elastic Computing Cloud
EGEE	Enabling Grids for e-Science
FTS	File Transfer Service
GEMLCA	Grid Execution Management for Legacy Code Applications
GIN-CG	Grid Interoperation Now Community Group
GLUE	Grid Laboratory Uniform Environment
GMT	Grid Monitoring Tool
GPFS	General Parallel File System
GRAM	Globus Resource Allocation Manager
GRIA	Grid Resources for Industrial Applications
GSM-WG	Grid Storage Management Working Group
HPC	High-Performance Computing
HPC-BP	HPC-Basic Profile
HPC-FSP	HPC-File Staging Profile
HTC	High Throughput Computing
IETF	Internet Engineering TaskForce

IGIIW	International Grid Interoperation and Interoperability Workshop
IGTF	International Grid Trust Federation
IVOM	Interoperability and Integration of VO Management Technologies
JDL	Job Description Language
JSDL	Job Submission Description Language
LCG	LHC Computing Grid
LDAP	Lightweight Directory Access Protocol
LDIF	LDAP Data Interchange Format
LHC	Large Hadron Collider
MD	Molecular Dynamics
MDS	Monitoring and Discovery Service
NAMD	Nanoscale Molecular Dynamics
NAREGI	National Research Grid Infrastructure
NDGF	Nordic DataGrid Facility
NGS	National Grid Service
NJS	Network Job Supervisor
OASIS	Organisation for the Advancement of Structured Information Standards
OGF	Open Grid Forum
OGSA	Open Grid Services Architecture
OGSA-BES	OGSA-Basic Execution Service
OGSA-DMI	OGSA-Data Movement Interface
OGSA-RUS	OGSA-Resource Usage Service
OGSI	Open Grid Services Infrastructure
OMII	Open Middleware Infrastructure Institute
OSG	Open Science Grid
PMA	Policy Management Authorities
PRAGMA	Pacific Rim Applications and Grid Middleware Assembly
RSL	Resource Specification Language
SAGA	Simple API for Grid Applications
SAML	Security Assertion Markup Language
SGAS	Swedish Grid Accounting System
SPMD	Single Program Multiple Data
SQL	Structured Query Language
SRB	Storage Resource Broker
SRM	Storage Resource Manager
TDDFT	Time-Dependent Density Functional Theory
TLS	Transport Level Security
UI	User Interface
UNICORE	Uniform Interface to Computing Resources
URF	Usage Record Format
URL	Uniform Resource Locator
UUDB	UNICORE User Database
VO	Virtual Organization
VOMS	VO Management Service

VM	Virtual Machine
W3C	World Wide Web Consortium
WISDOM	Wide In Silico Docking On Malaria
WN	Worker Node
WS	Web Services
WS-DAIR	WS Data Access and Integration Relational
WS-I	WS Interoperability
WS-RF	WS Resource Framework
XACML	Extensible Access Control Markup Language

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REFERENCES

1. OGF—Grid Interoperation Now Community Group (GIN–CG). http://forge.ogf.org/sf/projects/gin [2008].
2. OGF GLUE 2.0 Working Group. https://forge.gridforum.org/sf/projects/glue-wg [2008].
3. Australian Partnership for advanced computing (APAC). http://www.apac.edu.au/ [2008].
4. German National Grid D-Grid. http://www.d-grid.org [2008].
5. National Research Grid Initiative (NAREGI). http://www.naregi.org [2008].
6. National Grid Service (NGS). http://www.grid-support.ac.uk/ [2008].
7. Enabling Grid for e-Science (EGEE). http://public.eu-egee.org/ [2008].
8. Distributed Infrastructure for Supercomputing Applications (DEISA). http://www.deisa.org [2008].
9. Pacific Rim Applications and Grid Middleware Assembly (PRAGMA). http://www.pragma-grid.net/ [2008].
10. Nordic DataGrid Facility (NDGF). http://www.ndgf.org/ndgfweb/home.html [2008].
11. TeraGrid. http://www.teragrid.org/index.php [2008].
12. Open Science Grid. http://www.opensciencegrid.org/ [2008].
13. Foster I, Kesselman C, Tuecke S. The anatomy of the grid-enable scalable virtual organizations. *Grid Computing—Making the Global Infrastructure a Reality*. Wiley: New York, 2003; 171–198.
14. Rajasekar A, Wan M, Moore R, Schroeder W. A prototype rule-based distributed data management system. *Proceedings of the HPDC Workshop on Next Generation Distributed Data Mangagement*, Paris, France, 2006.
15. Shoshani A, Sim A, Gu J. Storage resource managers—essential components on the Grid. *Grid Resource Management*. Kluwer: Dordrecht, 2003.
16. Mandrichenko I, Allcock W, Perelmutov T. GridFTP v2 protocol description, GFD.47. http://www.ogf.org/documents/GFD.47.pdf [2005].
17. DMTF: Common Information Model (CIM) Standards. http://www.dmtf.org/standards/cim/ [2008].
18. Berkeley Database Information Index (BDII). https://twiki.cern.ch/twiki/bin/view/EGEE/BDII [2008].
19. Schopf JM, Raicu I, Pearlman L, Miller N, Kesselman C, Foster I, D'Arcy M. Monitoring and discovery in a web services framework: Functionality and performance of the globus toolkit's MDS4. *Technical Report ANL/MCS-P1248-0405*, Argonne National Laboratory, 2004.
20. Foster I, Grimshaw A, Lane P, Lee W, Morgan M, Newhouse S, Pickles S, Pulsipher D, Smith C, Theimer M. OGSA basic execution service, version 1.0, GFD.108. http://www.ogf.org/documents/GFD.108.pdf [2007].
21. OGF—OGSA-Resource Usage Service Working Group (OGSA-RUS). https://forge.gridforum.org/projects/rus-wg [2008].
22. GridToday: Striving for Grid interoperability now. http://www.gridtoday.com/grid/1918361.html [2008].
23. Open LDAP. http://www.openldap.org [2008].
24. Good G. The LDAP Data Interchange Format (LDIF)—Technical specification. http://www.ietf.org/rfc/rfc2849.txt [2008].
25. Grid Storage Management (GSM) Working Group. https://forge.gridforum.org/projects/gsm-wg/ [2008].

26. dCache. http://www.dcache.org/ [2008].
27. NAMD scalable molecular dynamics. http://www.ks.uiuc.edu/Research/namd/ [2008].
28. Santos N, Koblitz B. Distributed metadata with the AMGA metadata catalog. *Workshop on Next-generation Distributed Data Management*, HPDC-15, Paris, France, June 2006.
29. Antonioletti M, Collins B, Krause A, Laws S, Magowan J, Malaika S, Paton N. Web Services Data Access and Integration—The relational realisation (WS-DAIR) specification, version 1.0. GFD.76. http://www.ogf.org/documents/GFD.76.pdf [2006].
30. Laure E, Fisher SM, Frohner A, Grandi C, Kunszt PZ, Krenek A, Mulmo O, Pacini F, Prelz F, White J, Barroso M, Buncic P, Hemmer F, Di Meglio A, Edlund A. Programming the Grid with gLite. *Computational Methods in Science and Technology*. Scientific Publishers OWN: Poznan, Poland, 2006; 33–46.
31. Foster I. Globus toolkit version 4: Software for service-oriented science. *Proceedings of IFIP International Conference on Network and Parallel Computing* (*Lecture Notes in Computer Science*, vol. 3779). Springer: Berlin, 2005; 213–223.
32. Streit A *et al*. UNICORE—From project results to production grids. *Grid Computing*: *The New Frontiers of High Performance Processing* (*Advances in Parallel Computing*, vol. 14). Elsevier: Amsterdam, 2005; 357–376.
33. Wide In Silico Docking On Malaria (WISDOM). http://wisdom.eu-egee.fr/ [2008].
34. Foster I, Kesselman C, Tsudik G, Tuecke S. A security architecture for computational grids. *Fifth ACM Conference on Computer and Communications Security*. ACM: New York, 1998; 83–91.
35. Alfieri R, Cechini R, Ciaschini V, dell'Agnello L, Frohner A, L"orentey K, Spataro F. From gridmap-file to VOMS: Managing authorization in a grid environment. *Future Generation Computer Systems* 2005; **21**(4):549–558.
36. Stamou K, Hedman F, Iliopoulos A. Extending UNICORE 5 authentication model by supporting proxy certificate profile extensions. *UNICORE Summit 2007 in Conjunction with the European Conference on Parallel Computing 2007* (*Euro-Par2007*), Rennes, France, 2007.
37. Anjomshoaa A, Brisard F, Drescher M, Fellows D, Ly A, McGough S, Pulsipher D, Savva A. Job Submission Description Language (JSDL), specification v1.0. GFD.56. http://www.ogf.org/documents/GFD.56.pdf [2005].
38. Dillaway B, Humphrey M, Smith C, Theimer M, Wasson G. HPC basic profile, version 1.0, GFD.114. http://www.ogf.org/documents/GFD.114.pdf [2007].
39. Dierks T, Rescorla E. The Transport Layer Security (TLS) Protocol, version 1.1. http://tools.ietf.org/html/rfc4346 [2008].
40. Nadalin A, Kaler C, Monzillo R, Hallam-Baker Ph. OASIS WS-security username token profile 1.1. http://www.oasis-open.org/committees/download.php/16782/wss-v1.1-spec-os-UsernameTokenProfile.pdf [2008].
41. Open Middleware Infrastructure Institute for Europe (OMII-Europe). http://www.omii-europe.org [2008].
42. Venturi V, Stagni F, Gianoli A, Ceccanti A, Ciaschini V. Virtual organization management across middleware boundaries. *Proceedings of International Interoperation and Interoperability Workshop* (*IGIIW*) *2007*, Workshop at e-Science, Bangalore, India, 2007.
43. Piro RM, Guarise A, Werbrouck A. An economy-based accounting infrastructure for the DataGrid. *Proceedings of the Fourth International Workshop on Grid Computing*, Phoenix, 2003.
44. Sandholm T, Gardfjäll P, Elmroth E, Johnsson L, Mulmo O. A service-oriented approach to enforce grid resource allocation. *International Journal of Cooperative Information Systems* 2006; **15**:439–459.
45. Mach R, Lepro-Metz R, Jackson S, McGinnis L. Usage record—Format recommendation, GFD98. http://www.ogf.org/documents/GFD.98.pdf [2007].
46. Riedel M, Schuller B, Mallmann D, Menday R, Streit A, Tweddell A, Memon MS, Memon AS, Demuth B, Lippert Th, Snelling D, van den Berghe D, Li V, Drescher M, Geiger A, Ohme G, Benedyczak K, Bala P, Ratering R, Lukichev A. Web services interfaces and open standards integration into the European UNICORE 6 grid middleware. *Proceedings of 2007 Middleware for Web Services* (*MWS 2007*), *Workshop at the 11th International IEEE EDOC Conference 'The Enterprise Computing Conference'*, Annapolis, MD, U.S.A., 2007.
47. Frings W, Riedel M, Streit A, Mallmann D, van den Berghe S, Snelling D, Li V. LLview: User-level monitoring in computational grids and e-Science infrastructures. *Proceedings of German e-Science Conference 2007*, Baden-Baden, Germany, 2007.
48. Time-dependent density functional theory. http://www.tddft.org/ [2008].
49. The monitoring software for large scale grid system. http://www.opensce.org/components/SCMSWeb [2008].
50. Delaite T, Kiss T, Goyeneche A, Terstyszky G, Winter S, Kacsuk P. GEMLCA: Running legacy code applications as grid services. *Journal of Grid Computing* 2005; **3**(1–2), 75–90. Springer Science and Business Media B.V., Formerly Kluwer Academic Publishers B.V., ISSN 1570-7873.
51. Bitonti L, Kiss T, Terstynszky G, Delaite T, Winter S, Kacsuk P. Dynamic testing of legacy code resources on the grid. *Proceedings of the ACM International Conference on Computing Frontiers*, Ischia, Italy, 2–5 May 2006; 261–268.
52. Kacsuk P, Kiss T, Sipos G. Solving the grid Interoperability problem by P-GRADE portal at workflow Level. *Proceedings of the GELA Workshop at the 15th IEEE International Symposium on High Performance Distributed Computing* (*HPDC-15*), Paris, France, 2006.
53. Kacsuk P, Sipos G. Multi-grid, multi-user workflows in the P-GRADE portal. *Journal of Grid Computing* 2006; **3**(3–4):221–238.

54. Riedel M, Memon AS, Memon MS, Mallmann D, Streit A, Wolf F, Lippert Th, Venturi V, Andreetto P, Marzolla M, Ferraro A, Ghiselli A, Hedman F, Zeeshan A, Shah Salzemann J, Da Costa A, Breton V, Kasam V, Hofmann-Apitius M, Snelling D, van de Berghe S, Li V, Brewer S, Dunlop A, De Silva N. Improving e-Science with Interoperability of the e-Infrastructures EGEE and DEISA. *Proceedings of the 31st International Convention MIPRO*, *Conference on Grid and Visualization Systems* (*GVS*), Opatija, Croatia, Croatian Society for Information and Communication Technology, Electronics and Microelectronics, May 2008; 225–231. ISBN 978-953-233-036-6.
55. International Grid Trust Federation (IGTF). http://www.gridpma.org/ [2008].
56. Farrell S, Housley R. An internet attribute certificate profile for authorization. http://www.ietf.org/rfc/rfc3281.txt [2008].
57. OASIS—Security Services Technical Committee, Security Assertion Markup Language (SAML). http://www.oasis-open.org/committees/security [2008].
58. OASIS—Extensible Access Control Markup Language (XACML) Technical Committee. http://www.oasis-open.org/committees/xacml [2008].
59. OGF—OGSA-Data Movement Interface Working Group (OGSA-DMI). https://forge.gridforum.org/sf/projects/ogsa-dmi-wg [2008].
60. Wasson G, Humphrey M. HPC file staging profile, version 1.0, GFD.135. http://www.ogf.org/documents/GFD.135.pdf [2008].
61. European and Chinese Cooperation on the Grid. http://echogrid.ercim.org/ [2008].
62. India's National Grid Computing Initiative. http://www.garudaindia.in [2008].
63. Wang Y, Scardaci D, Yan B, Huang Y. Interconnect EGEE and CNGrid e-Infrastructures through interoperability between gLite and GOS middleware. *International Grid Interoperability and Interoperation Workshop* (*IGIIW 2007*), *Third IEEE International Conference on e-Science and Grid Computing*, Bangalore, India, 2007; 553–560.
64. German IVOM Project. http://dgi.d-grid.de/index.php?id=314 [2008].
65. Tunisian Grid (GTRS). http://www.esstt.rnu.tn/utic/gtrs/ [2008].
66. European BRIDGE Project. http://www.bridge-grid.eu [2008].
67. Amazon's Elastic Compute Cloud (EC2). http://aws.amazon.com/ec2/ [2008].