Improving e-Science with Interoperability of the e-Infrastructures EGEE and DEISA

Morris Riedel, A.S. Memon, M.S. Memon, Daniel Mallmann,
Achim Streit, Felix Wolf, and Thomas Lippert
Jülich Supercomputing Centre, Forschungszentrum Jülich (FZJ), Leo-Brandt-Str. 1, Jülich, 52425, Germany
Phone: (+49) 02461 61 - 3651 Fax: (+49) 02461 61 6656 E-mail: m.riedel@fz-juelich.de

Valerio Venturi, Paolo Andreetto, Moreno Marzolla, Andrea Ferraro, Antonia Ghiselli
INFN-CNAF, INFN-Padova, National Institute of Nuclear Physics (INFN), Italy

Fredrik Hedman, Zeeshan Ali Shah
Center for Parallel Computers (PDC), Royal Institute of Technology (KTH), Sweden

Jean Salzemann, Ana Da Costa, Vincent Bloch, Vincent Breton
Laboratoire de Physique Corpusculaire, Clermont-Ferrand (LPC), France

Vinod Kasam, Martin Hofmann-Apitius
Fraunhofer SCAI, Germany

David Snelling, Sven van de Berghe, Vivian Li
Fujitsu Laboratories Europe (FLE), UK

Steve Brewer, Alistair Dunlop, Nishadi De Silva
University of Southampton, UK

Abstract – In the last couple of years, many e-Science infrastructures have begun to offer production services to e-Scientists with an increasing number of applications that require access to different kinds of computational resources. Within Europe two rather different multi-national e-Science infrastructures evolved over time namely Distributed European Infrastructure for Supercomputing Applications (DEISA) and Enabling Grids for E-SciencE (EGEE). DEISA provides access to massively parallel systems such as supercomputers that are well suited for scientific applications that require many interactions between their typically high numbers of CPUs. EGEE on the other hand provides access to a world-wide Grid of university clusters and PC pools that are well suited for farming applications that require less or even no interactions between the distributed CPUs. While DEISA uses the HPC-driven Grid technology UNICORE, EGEE is based on the gLite Grid middleware optimized for farming jobs. Both have less adoption of open standards and therefore both systems are technically non-interoperable, which means that no e-Scientist can easily leverage the DEISA and EGEE infrastructure with one suitable client environment for scientific applications. This paper argues that future interoperability of such large e-Science infrastructures is required to improve e-Science in general and to increase the real scientific impact of world-wide Grids in particular. We discuss the interoperability achieved by the OMII-Europe project that fundamentally improved the interoperability between UNICORE and gLite by using open standards. We also outline one specific scientific scenario of the WISDOM initiative that actually benefits from the recently established interoperability.

I. INTRODUCTION

In the past several years, many scientific applications from various domains have taken advantage of e-Science infrastructures that share storage or computational resources. Various e-Science infrastructures exist today (e.g. EGEE [1], OSG [2], PRAGMA [3], TeraGrid [5]) already leading to new insights in scientific scenarios, but most of them will face new challenges during the coming years. The increasing complexity of Grid applications that embrace multiple physical models (i.e. multi-physics) and consider a larger range of scales (i.e. multi-scale) is creating a steadily growing demand for compute power and thus connected storage facilities.

Also, disproportional power dissipation and diminishing returns from additional instruction-level parallelism are limiting further progress in uni-processor performance. Therefore, the only option left to satisfy increasing Grid application demands is to harness higher degrees of parallelism by employing a larger number of moderately fast processor cores on a single chip (i.e., multi-core). This will especially influence supercomputer Grids such as DEISA [4] in the near future that will have to integrate peta-scale computers with millions of CPUs.

However, the integration of such large-scale computing resources as well as the usage of more and more complex multi-physics applications will pose major challenges. First and foremost, e-Scientists require access to the different kinds of computational resources (Supercomputers vs. PC pools) while there is no common way of doing this today. For instance, while one part of the scientific workflow actually requires massively parallel systems with an application that is based on the Message Passing Interface (MPI) [6], another part of the scientific workflow is just a farming application that does not need costly CPU time on massively parallel systems. Hence, e-Scientists require one technology to access these different systems in a seamless way without being a Grid expert. They actually require Grid technologies that are interoperable and provide easy access to their different kinds of e-Science infrastructures.

Based on the GEANT network infrastructure within Europe, there are two different kinds of e-Science infrastructures namely Enabling Grids for e-Science (EGEE) [1] and Distributed European Infrastructure for Supercomputing Applications (DEISA) [4]. While DEISA is a supercomputing infrastructure that consists of systems that allow for MPI-based massively parallel jobs, the EGEE infrastructure is well suited for farming and rather embarrassingly parallel applications that require less or even no interactions between the CPUs.

The fundamental challenges in interoperability between these infrastructures rely on the different technologies that provide access to them. DEISA uses the UNICORE 5 Grid technology [7] in production and is in the process of evaluation of the UNICORE 6 technology [8] that is based on Web services (WS). EGEE, on the other hand, is based on gLite [9], which will integrate numerous recent developed WS components as well in the near future. Both deployed Grid technologies are currently not technically interoperable. This means that no e-Scientist can conveniently use the DEISA infrastructure in conjunction with EGEE for applications during one scientific workflow although it is required during some scientific scenarios.

In this paper we define long-term interoperability as the ability of Grid technologies to interact via emerging common open standards. Interoperation, on the other hand, is defined as what needs to be done to get Grids to work together as a fast short-term achievement using as much existing technologies as available. Many examples of these interoperation efforts are conducted within the Grid Interoperation Now (GIN) community group [34] of OGF.

To ensure that both Grid technologies, UNICORE and gLite, are technically interoperable in the near future, the Open Middleware Infrastructure Institute for Europe (OMII-Europe) project [10] is funded by the EU to significantly influence the adoption and development of open standards in both technologies. We define open standards as emerging mature specifications (i.e. OGF recommendations) that have the potential to become a full accepted standard very soon. Therefore, both middleware systems have been augmented with numerous open standards that facilitate interoperability between them such as OGSA – Basic Execution Services (BES) [11] and Job Submission Description Language (JSDL) [12].

In addition, the project developed and established a Common Security Profile (CSP) that enables these middleware systems to interact in a secure way by using a fixed set of security specifications. Among others, the most important specifications are transport layer security (TLS) and the Security Assertion Markup Language (SAML) [25]. Also, the CSP implies that attribute-based authorization (i.e. attributes such as roles and capabilities) is a natural requirement of e-Science infrastructures instead of using plain identity-based authorization (i.e. only X.509 certificates). An interesting fact is that the implemented components are in process of adoption by the Grid middleware providers, which means that there is a very high chance that the interoperability components will be soon deployed on infrastructures such as DEISA or EGEE.

In this paper we will shortly outline the difference between the currently deployed proprietary interfaces of UNICORE and gLite. This is necessary to understand the major contribution of this paper discussing the recently developed interoperability of UNICORE and gLite in the context of a real scientific scenario out of the WISDOM initiative [13]. Of course, the scenario describes a technical interoperability between gLite and UNICORE enabled by the OMII-Europe project, but it is worth mentioning that the actual usage of the DEISA and EGEE infrastructures as described within this contribution is still subject to the scientists to negotiate with the respective infrastructures.

This paper is structured as follows. After reviewing the difference between UNICORE and gLite in Section 2, Section 3 will discuss how both systems can be used to submit scientific jobs to different kinds of infrastructures using OMII-Europe components. Section 4 will provide an overview of other types of scientific scenarios that can leverage the proposed interoperability between Grids. Finally, after surveying related work in Section 5, we present our conclusion in Section 6.

II. The UNICORE and gLite Grid Technologies

The Uniform Interface to Computing Resources (UNICORE) Grid technology [7] provides a seamless, secure, and intuitive access to distributed Grid resources such as supercomputers, clusters, or server-farms. The non Web services-based UNICORE 5 system is used in daily production at supercomputer centers and research facilities world-wide today. Beyond this production usage, e.g. within the European DEISA infrastructure or national Grid initiatives like the German D-Grid [14] or Swiss Grid Initiative [15], it serves as a solid basis in many European and International research projects such as OMII-Europe, A-Ware [16] and Chemomentum [17].

UNICORE is developed since 1997 and thus it incorporates numerous proprietary protocols and interfaces since the open standards of the Open Grid Forum (OGF) are only emerging slowly over the last years, especially in the context of job submission. Therefore, UNICORE is based on a proprietary UNICORE Protocol Layer (UPL) [7] and uses proprietary job descriptions named as Abstract Job Objects (AJOs) [7]. Since UNICORE is mostly used at HPC centers, the concept of Virtual Organizations (VOs) is not integrated in UNICORE 5 as well, because in most of the HPC centers the access based on VOs is rather contrary to their typical access paradigms (e.g. based on typical UNIX user accounts instead of dynamic VO accounts).

The gLite Grid middleware [9] supports large distributed computing environments such as the EGEE infrastructure and consists of many types of technologies for various tasks within a Grid. In contrast to UNICORE where an end-user explicitly chooses a supercomputer for a scientific job submission, in gLite the Workload Management System (WMS) [9] basically acts as a resource broker and submits a job to a computational resource that provides the amount of free CPUs that are required. Another major difference between UNICORE and gLite is that UNICORE use full X.509 certificates while gLite is using X.509 proxies with embedded information about VO membership, known as Virtual Organization Membership Service (VOMS) [18] proxies (i.e. attribute certificates).

In terms of job submission, gLite is based on rather proprietary protocols such as the Job Definition Language (JDL) [9]. JDL is used to submit to the WMS that forwards submissions to the computing elements. The most recent computing element in gLite is the Computing Resource Execution and Management (CREAM) [19] system that is designed to provide efficient processing of a large number of requests for computation on managed resources in EGEE. CREAM accepts a request from distributed clients using Web services technologies and the architecture is designed to be robust, scalable and fault tolerant.

To sum up, both Grid technologies rely on different security models and provide proprietary interfaces in terms of job submission and description. All in all, this makes it really difficult to use one client to access both systems. However, these differences and the requirement of interoperability within scientific scenarios on European e-Science infrastructures motivated the establishment of the OMII-Europe project that focuses on interoperability between these systems using open standards.

III. Interoperability between UNICORE and gLite

A. Improving e-Science with Grid Interoperability

While the developed components of OMII-Europe can be used for many different interoperability scenarios we provide here a real world example in the context of the WISDOM initiative [13]. WISDOM aims at developing new drugs for Malaria and so far WISDOM scientists have used the EGEE e-Science infrastructure for large-scale in-silico docking methods and their scientific workflows. An overview of this interoperability scenario is shown in Fig. 2, while the scientific workflow steps are marked with numbers from (1) to (9).

In particular, the scientific applications FlexX [20] and AutoDock [21] are used and typically provided on several resources within the EGEE infrastructure accessible via gLite. However, the output is only a list of best chemical compounds that are potential drugs and thus not the final solution. Therefore, a scientific method developed by G. Rastelli et al. [22] is to use molecular dynamics (MD) computations to refine this best compound list. While this step was so far done on the EGEE e-Infrastructure, there is a lot of potential to use the scalable Assisted Model Building with Energy Refinement (AMBER) [23] molecular dynamics package within the DEISA e-Science infrastructure with highly scalable supercomputers.

Therefore, the fundamental goal of this interoperability scenario is to improve the e-Science methods in the WISDOM initiative and thus significantly accelerate the drug discovery process by using EGEE in conjunction with DEISA by exploiting the OMII-Europe interoperability components for their respective Grid middlewares. In more detail, the interoperability scenario demonstrates how OMII-Europe components are used to enable interoperability between the open standard-compliant UNICORE 6 Grid middleware and CREAM-BES of gLite that are both currently being analyzed for the deployment in the e-Science infrastructures DEISA and EGEE.

The interoperability of these systems has been reached by adopting the same open standards such as the OGSA – Basic Execution Services (BES) [11] and Job Submission Description Language (JSDL) [12]. Since security is crucial for interoperability as well both systems agreed to the same security setup that we defined as Common Security Profile (CSP). In fact this security profile is suitable for production scenarios within e-Science infrastructures, including standards like IETF Transport Layer Security (TLS) [24] as well as VO management based on the SAML standard released by the Organization of Advancement of Structured Information Standards (OASIS).

B. e-Scientists require an Interoperable Client Technology

Within current European e-Infrastructures such as EGEE and DEISA, the scientists use a dedicated Grid client to access their respective Grid middleware systems gLite and UNICORE as shown in Fig 1. OMII-Europe also works on providing a GridSphere portal [26] that accesses both Grid middleware systems, but in general, any other Grid middleware client that is compliant with the CSP is able to access them.

While gLite provides a command-line client, UNICORE, so far, is rather oriented towards GUI clients. Recently, the OMII-Europe project developed several plug-ins for the Eclipse-based UNICORE Rich Client Platform (RCP) in order to not only access UNICORE but also any other middleware that is compliant with open standards such as OGSA-BES and SAML-based VOMS. Since CREAM-BES of gLite is compliant to those standards, we can use the UNICORE RCP client to submit scientific jobs also to this system as shown in Fig. 1.

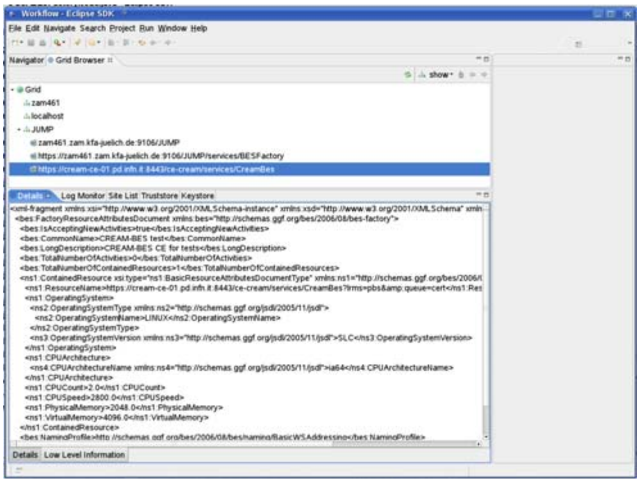

Fig. 1. The Eclipse-based UNICORE Rich Client Platform with OGSA-BES Plug-ins that are able to access any standard compliant Grid middleware that agrees to the same CSP. This Figure shows the access via UNICORE to the Supercomputer JUMP in DEISA and access via CREAM-BES to an EGEE site.

Hence, the OGSA-BES plug-in of the UNICORE RCP client can be used to access any OGSA-BES compliant Grid middleware; however, the security setup is crucial as well. Therefore, the OMII-Europe project developed the

CSP and the recently developed SAML-based VOMS system is one cornerstone of this profile. Another important plug-in of the UNICORE RCP client is able to request SAML assertions for end-users from a SAML-based VOMS server [27]. Such assertions are shipped with the OGSA-BES CreateActivity() [11] operation request inside the SOAP header [28] and thus can be used for authorization within OGSA-BES compliant Grid middleware, which supports the authorization based on SAML assertions. In terms of authentication we rely on typical X.509 certificates signed by a trusted Certificate Authority (CA) that are also being used for TLS by the client.

C. Scientific Workflow with Interoperable Components

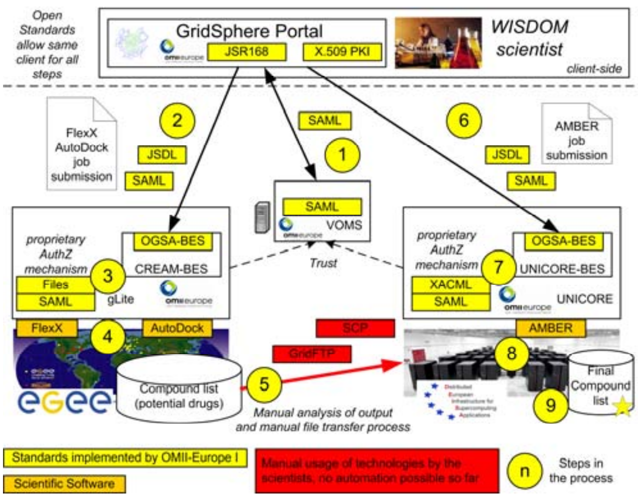

Fig. 2. Overview of the scientific interoperability scenario WISDOM that requires resources in EGEE and DEISA.

The overall scientific workflow is initiated by an e-Scientist that uses the UNICORE RCP client (or a GridSphere portal) to request a SAML assertion from the VOMS service of the corresponding VO. This workflow step is marked as (1) within Fig. 2. The server, in turn releases a signed SAML assertion stating the identification and role possession of the e-Scientist within a group or project.

As shown in Fig.1, within workflow step (2), a GridSphere portal uses the assertion during an OGSA-BES compliant job submit using JSDL. The JSDL describes the invocation of scientific applications that are defined by the e-Scientists. The parameters for the applications are also coded within the JSDL description. In our example scenario, the scientific applications FlexX and AutoDock are being used on embarrassingly parallel systems within the EGEE e-Infrastructure.

As part of gLite in the near future, the CREAM-BES service is using the JSDL document to invoke the FlexX and AutoDock applications with the CREAM backend on the EGEE e-Infrastructure. In more detail the CreateActivity() operation of the CREAM-BES OGSA-BES implementation takes a JSDL as input that is then further analyzed by CREAM-BES for job execution. This step is indicated as (3) within Fig. 2. Right before this job execution, the authorization layer within CREAM-BES checks whether the SAML assertion allows the end-user (i.e., e-Scientist) to execute applications on the infrastructure.

In workflow step (4), FlexX and/or AutoDock are computed on the EGEE infrastructure as embarrassingly parallel scientific applications that require no interactions between the processes on different CPUs. The outcome of this computational intensive job is an intermediary result in terms of a compound list that represents potential drugs. It is stored by using the typical storage mechanisms of gLite.

In order to use these intermediary results of the EGEE job outcome within the DEISA infrastructure, the data must be transferred to DEISA storage systems at the corresponding supercomputer site. This can be done manually using GridFTP [29] or SCP since these steps require a manual intervention from the e-Scientists. Hence, the scientific process requires that scientists analyze the outcome of the EGEE jobs and take particular ones as input for the DEISA jobs. This rather manual transfer workflow step is marked with (5) in Fig. 2.

Assuming that the data of the intermediary results are reachable within DEISA, the WISDOM e-Scientists uses again the UNICORE RCP client to submit another JSDL-compliant job to the UNICORE OGSA-BES interface implementation installed at some supercomputer site within the DEISA infrastructure. As shown in workflow step (6) in Fig. 2, the JSDL describes the execution of a highly scalable AMBER c/fortran script code within DEISA. Again, the (not necessarily same) SAML assertion must be transferred during the job submit to ensure the authorization of the e-Scientist later within the UNICORE authorization layer.

Workflow step (7) in Fig. 2 shows that the UNICORE OGSA-BES implementation is using the JSDL document to invoke the AMBER application via UNICORE, taking the parameters defined in JSDL into account. The OGSA-BES implementation in UNICORE is using the same execution backend as the proprietary interfaces and thus enables a job submit to resource management systems of supercomputers. However, before this application can be finally started on the DEISA infrastructure, an authorization of the e-Scientist must be performed by using the SAML assertion in conjunction with the eXtensible Access Control Markup Language (XACML) [30] policy checks in the UNICORE execution backend. This backend is named as the Network Job Supervisor (NJS) [8], which in turn forwards jobs to Target System Interfaces (TSI) [8].

The AMBER application is computed on the DEISA infrastructure on massively parallel supercomputers. This MD script was developed by G. Rastelli et al. [22] and is executed by using typical JSDL descriptions. The script itself uses several different programs of the AMBER molecular dynamics package (e.g. ptray, sander, etc.). This step is now significantly faster than without the interoperability between EGEE and DEISA, because the AMBER code is highly scalable and thus capable of leveraging the massive number of CPUs available on resources within the DEISA infrastructure. The outcome of this job is the final result. This step is marked with (8) in Fig. 2.

Finally, by using UNICORE on DEISA the outcome of this job, which is the final compound list, can be obtained using again the UNICORE RCP client. All in all, the workflow steps described a scientific solution that has been computed within EGEE and DEISA and would not be possible without interoperable components of OMII-Europe.

IV. Other Interoperability Scenarios

The interoperability scenario mentioned in Section 3 represents only one particular class of interoperability use cases that can leverage the interoperability between UNICORE and gLite. Of course, the OMII-Europe project developed more components that can be used in numerous other classes of interoperability use cases.

One particular example is the collaboration with EU-IndiaGrid project [31] and the interoperability between the Indian national Grid GARUDA [32] and European e-Science Infrastructures. The fundamental aim of this collaboration is to setup a computational research environment for quantum atomistic simulations that can seamlessly access the different Grid infrastructures GARUDA, EGEE, and DEISA for different kind of calculations. Quantum atomistic simulations are very demanding in terms of CPU and memory requirements.

In more detail, the GARUDA infrastructure is based on Globus Toolkit 4 [33], which also developed its own job description language named as Resource Specification Language (RSL) [33]. The Globus Grid Resource Allocation Manager (GRAM) [33] component takes RSL job descriptions via a proprietary job submission interface. In this context, the OMII-Europe project also developed in collaboration with the Globus developers in USA the Globus OGSA-BES implementation, which uses the JSDL standard for job description. In more detail, the OGSA-BES implementation is used as another job submission interface to the Globus WS-GRAM component.

The scientific process in this scenario is as follows. The scientists that do quantum atomistic research use the VASP and Wien2k scientific applications that are well known and already ported on all three e-Science infrastructures GARUDA, EGEE and DEISA. The different Grids are used for different scales of application demands increasing from the national GARUDA Grid over EGEE towards the Supercomputing DEISA Grid.

To sum up, the scientists prepare jobs for different kinds of systems and different types of scales ranging from small systems for parameter sweep studies to big systems with many-core CPUs for full blown production runs. By using the job submission interface OGSA-BES and JSDL as job description language one suitable client can securely submit jobs seamlessly to UNICORE, gLite and Globus.

V. Related Work

One famous project in the context of interoperability was the Grid Interoperability Project (GRIP) [35] that achieved interoperability between the non WS-based UNICORE 5 and the non WS-based Globus Toolkit 2.4. In short, UNICORE 5 has been extended to support proxies to achieve the necessary interoperability on the security layer. For interoperable job submission the UNICORE 5 system was enhanced with a specific Target System Interface (TSI) [7] to submit to a Globus pre-WS GRAM system. All in all, this interoperability worked well, but with the evolution of both systems towards WS-based systems, the reached interoperability was not longer applicable.

Another related work within the EGEE-II project is based on the interoperation between UNICORE 5 and production gLite to enable the systems to simply interoperate without using any job submission and management standard. In particular, the WMS is tweaked with a special option to submit gLite jobs to a special computing element that in facts represent a UNICORE installation if necessary.

A submit from UNICORE to gLite, on the other hand, is processed through the complete UNICORE stack but then forwarded to a Target System Interface (TSI) that submits a job into the gLite system through the gLite user interface. While there is collaboration between OMII-Europe and the EGEE-II project in this matter, this rather short-term achievement works only with a specific version of UNICORE 5 and with a specific version of gLite, while we provide with the approach described within this paper a longer-term solution by using common open standards of OGF and OASIS. Particular benefits of our approach are sustainability of the interoperability as well as the avoidance of processing one job in the first stack completely before submitting the job to the other middleware stack.

Another well known work in the field of related work is the GIN [34] activity within the OGF where a member of OMII-Europe project took the active role as Secretary and later as co-chair. In this group, many production Grids regularly interact with other Grids in a pair wise fashion, e.g. cross-Grid job information exchange. Nevertheless these single interoperation efforts are much different from native interoperability as described within this contribution.

Finally, there is interoperability work from the team of the P-Grade portal [36] that also tries to bridge different Grid and e-Science infrastructures by providing access to standards-based interoperable middleware. However, we distinguish our approach from this by the fact that the components of OMII-Europe are fed back into the middleware systems UNICORE, gLite and Globus.

VI. CONCLUSION

We described the technical interoperability between EGEE and DEISA by providing interoperability components for their respective Grid middleware technologies UNICORE and gLite. The interoperability components that have been developed by the OMII-Europe project have the potential to be used in real scientific scenarios such as the WISDOM initiative or EU-IndiaGrid scientific use cases once they are finally deployed.

While scientific results will be published in the respective community journals we can state that the interoperability scenario accelerates the drug discovery process and thus it indicates that interoperability through open standards is a feasible approach, also for production e-Science infrastructures such as DEISA and EGEE.

The here described solution is not only applicable within

DEISA and EGEE, because also other national and international Grids are using the gLite and UNICORE technologies. To provide an example, the German national Grid D-Grid uses gLite, UNICORE and Globus for the access of computational resources. Hence, the achieved interoperability of gLite, Globus and UNICORE with respect to job submission and management is also very useful for this production e-Science infrastructure. Furthermore, it is important to understand that the described interoperability between UNICORE 6 and CREAM-BES of gLite is not tailored to specific versions of them or tailored for these Grid middlewares. In principle, any Grid technology that is capable of providing support for the same common security profile and open standards is interoperable with UNICORE and gLite.

Finally, it is important to mention that UNICORE 6 and CREAM-BES of gLite as well as the SAML VOMS server are still in the process of evaluation and thus not yet deployed on the e-Science infrastructures DEISA and EGEE today. However, since the middleware providers of these systems have been part of the developing project OMII-Europe, it is expected that the interoperability components will be integrated in the major releases and thus soon deployed in any infrastructures that would like to use these Grid middleware systems in interoperable world-wide Grids.

ACKNOWLEDGMENTS

The work presented in this paper has been supported by the OMII-Europe project under EC grant RIO31844-OMII-EUROPE, duration May 2006 – April 2008.

REFERENCES

[1] Enabling Grids for E-Science project, http://www.eu-egee.org/

[2] Open Science Grid (OSG) Project, http://www.opensciencegrid.org/

[3] Pacific Rim Applications and Grid Middleware Assembly (PRAGMA), http://www.pragma-grid.net/

[4] Distributed European Infrastructure for Supercomputing Applications (DEISA), http://www.deisa.org

[5] TeraGrid, http://www.teragrid.org/

[6] P. Pacheco, *"Parallel Programming with MPI"*, Morgan Kaufmann, 1996, ISBN 1558603395.

[7] A. Streit et al., *"UNICORE – From Project Results to Production Grids"*, In L.Grandinetti, editor, Grid Computing: The New Frontiers of High Performance Processing, Advances in Parallel Computing 14, pages357-376, Elsevier.

[8] M. Riedel et al., *"Web Services Interfaces and Open Standards Integration into the European UNICORE 6 Grid Middleware"*, In Proceedings of the 2007 Middleware for Web Services (MWS 2007), Workshop at 11th International IEEE EDOC Conference "The Enterprise Computing Conference", 2007, Annapolis, Maryland, USA.

[9] E. Laure et al., *"Programming the Grid with gLite"*, In Computational Methods in Science and Technology, pages 33 – 46, Scientific Publishers OWN, 2006

[10] Open Middleware Infrastructure Institute for Europe (OMII-Europe), http://www.omii-europe.org

[11] I. Foster et al., *"OGSA – Basic Execution Services"*, In OGF Grid Final Documents No. 108

[12] A. Anjomshoaa et al., *"Job Submission Description Language (JSDL) Specification v1.0"*, In OGF Grid Final Documents No. 56

[13] Wide In Silicio Docking on Malaria (WISDOM) Initiative, http://wisdom.healthgrid.org/

[14] German National Grid D-Grid, http://www.d-grid.de/

[15] Swiss Grid Initiative, http://www.gridinitiative.ch/middleware.html

[16] An Easy Way to Access Grid Resources (A-Ware), http://www.a-ware-project.eu/

[17] Chemomentum Project, http://www.chemomentum.org/c9m

[18] R. Alfieri et al., *"From gridmap-file to voms: managing authorization in a Grid"*, In Future Generation Comp. Systems, 21(4), 2005, pages 549- 558.

[19] P. Andreetto et al., *"CREAM: A simple, Grid-accessible Job Management System for local Computational Resources"*, In CHEP 2006, Mumbay, India, 2006.

[20] FlexX, http://www.biosolveit.de/FlexX/

[21] AutoDock, http://autodock.scripps.edu/

[22] G. Rastelli et al., *"Validation of an automated procedure for the prediction of relative free energies of binding on a set of aldose reductase inhibitors"*, In Bioorg Med Chem, 2007 Dec. 15, 15(24), 7865-77, Epub 2007.

[23] Assisted Model Building with Energy Refinement (AMBER), http://amber.scripps.edu/

[24] Transport Layer Security, IETF RFC 4346, http://tools.ietf.org/html/rfc4346

[25] OASIS Security Services (SAML) TC, http://www.oasisopen.org/committees/security.

[26] GridSphere Portals, http://www.gridsphere.org/gridsphere/gridsphere

[27] V. Venturi et al., *"Using SAML-based VOMS for Authorization within Web Services-based UNICORE Grids"*, In Proceedings of 3rd UNICORE Summit 2007 in conjunction with EuroPar 2007, Rennes, France.

[28] Simple Object Access Protocol (SOAP), W3C, http://www.w3.org/TR/soap/

[29] I. Mandrichenko et al., *"GridFTP v2 Protocol Description"*, In OGF Grid Final Documents No. 47

[30] OASIS XACML Technical Committee, http://www.oasis-open.org/committees/xacml

[31] EU-IndiaGrid, http://www.euindiagrid.eu/

[32] GARUDA, http://www.garudaindia.in/

[33] I. Foster et al., *"Globus Toolkit version 4: Software for Service-Oriented Science"*, In Proceedings of IFIP International Conference on Network and Parallel Computing, LNCS 3779, pages 213-223, Springer Verlag 2005

[34] Open Grid Forum (OGF) GIN Community Group, https://forge.gridforum.org/sf/projects/gin

[35] GRIP Project, http://www.ist-world.org/ProjectDetails.aspx?ProjectId=ec484bc8b17141058adfcaa26487a376

[36] Kacsuk P., Kiss T., Sipos G., *"Solving the Grid Interoperability Problem by P-GRADE Portal at Workflow Level"*, Proc. of the GELA Workshop at the 15th IEEE International Symposium on High Performance Distributed Computing (HPDC-15), Paris, France, 2006