Making distributed computing infrastructures interoperable and accessible for e-scientists at the level of computational workflows

Tamas Kiss

School of Electronics and Computer Science

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Abstract

As distributed computing infrastructures evolve, and as their take up by user communities is growing, the importance of making different types of infrastructures based on a heterogeneous set of middleware interoperable is becoming crucial. This PhD submission, based on twenty scientific publications, presents a unique solution to the challenge of the seamless interoperation of distributed computing infrastructures at the level of workflows.

The submission investigates workflow level interoperation inside a particular workflow system (intra-workflow interoperation), and also between different workflow solutions (inter-workflow interoperation). In both cases the interoperation of workflow component execution and the feeding of data into these components workflow components are considered.

The invented and developed framework enables the execution of legacy applications and grid jobs and services on multiple grid systems, the feeding of data from heterogeneous file and data storage solutions to these workflow components, and the embedding of non-native workflows to a hosting meta-workflow. Moreover, the solution provides a high level user interface that enables e-scientist end-users to conveniently access the interoperable grid solutions without requiring them to study or understand the technical details of the underlying infrastructure. The candidate has also developed an application porting methodology that enables the systematic porting of applications to interoperable and interconnected grid infrastructures, and facilitates the exploitation of the above technical framework.

Statement

I hereby declare that the submitted thesis is my own work. My contribution in the submitted papers is clearly specified in the commentary, and well differentiated from the co-authors of the papers.

Tamas Kiss, London, 16th July 2012

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Completing this PhD thesis has been a long and not always straightforward journey. Many people supported and encouraged me during this work and I would like to take this opportunity to acknowledge their contribution and to say thank you for their support.

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I would like to thank various colleagues at the Centre for Parallel Computing research group who worked with me during the years, influenced my ideas about the directions of the research, and provided me help in making these ideas happen. Dr Thierry Delaitre was always around when technical support or advice was needed. Many other colleagues, including Ariel Goyeneche, Gabor Kecskemeti, Szabolcs Illes, Tamas Kukla, Daniel Farkas, Alexandru Tudose, Gabor Szmetanko, Zsolt Lichtenberger and Noam Weingarten worked with me on various research topics resulting in papers comprising this submission.

Dr Pamela Greenwell has taught me an awful lot about molecules, proteins and ligands, and always reminded me to produce systems that are usable for scientists and end-users.

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2. **Tamas Kiss**, Gabor Terstyanszky, Gabor Kecskemeti, Szabolcs Illes, Thierry Delaittre, Stephen Winter, Peter Kacsuk, Gergely Sipos : *Legacy Code Support for Production Grids*
3. **Tamas Kiss**, Gergely Sipos, Peter Kacsuk, Krisztian Karoczkai, Gabor Terstyanszky, Thierry Delaitre: *Integration of GEMLCA and the P-GRADE Portal*
4. Luigi Bitonti, **Tamas Kiss**, Gabor Terstyanszky, Thierry Delaitre, Stephen Winter, Peter Kacsuk, *Dynamic Testing of Legacy Code Resources on the Grid*
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19. **Tamas Kiss**, Ian Kelley, Peter Kacsuk, Porting Computation and Data Intensive Applications to Distributed Computing Infrastructures Incorporating Desktop Grids
20. **Tamas Kiss,** et al: New Methodology to Create and Grid-enable Grid and Desktop Grid Applications

1. Introduction

Many scientific and business applications require extensive computational and data resources to run efficiently. Molecular docking simulations (e.g. as described in Heindl H. et al 2009) widely utilised by bio-scientist researchers and the pharmaceutical industry, take days or even weeks to complete on a standalone computer. Optimisation algorithms and risk analysis programs (e.g. as described in Kacsukne B. L. and Cselenyi J. 2005), used by businesses, banks and other financial institutions could be both data and computation intensive. Simulating traffic of a large city (e.g. as described in Kalantery N. et al 2003) requires large computing power and access to a huge amount of data. Examples can be given from practically all areas of science and business.

Research in grid and cloud computing infrastructures during the past decade resulted in production level resources that can be utilised to solve the above mentioned problems more quickly and efficiently. Resources are now available for scientists and companies to run computationally intensive experiments and to access large distributed data collections.

Examples of production level grid infrastructures include the European Grid Infrastructure, the EGI Grid (EGI 2011), or the TeraGrid (TeraGrid 2011) and Open Science Grid (OSG 2011) in the United States. These grids connect large computing clusters and/or supercomputers to serve scientific research. In a different approach, desktop computers of individuals or institutions are connected to large desktop or volunteer grid systems. The SETI@home project (Anderson D. P. et al 2002) is a prominent example for a global volunteer desktop grid, while the University of Westminster has connected all its laboratory computers into a local desktop grid system. The latest flavour of large scale production level computing and data resources are offered by commercial cloud computing providers, including Amazon or Google for example, who offer applications, tools and platforms on a pay as you go basis in a virtualised manner. These production infrastructures enable the construction and execution of applications and experiments on a previously unimagined scale triggering even more resource intensive scenarios.

Unfortunately, the above mentioned distributed computing infrastructures (DCIs) are provided as non-interoperable "production islands" causing difficulties when the experiment overgrows the capabilities of one specific DCI, or require access to a more heterogeneous set of resources. Different production infrastructures are based on different middleware, use different tools and policies for authentication and authorisation, describe and submit jobs differently, and provide data services based on a variety of protocols and access mechanisms. The utilisation of resources spreading over multiple DCIs based on heterogeneous solutions is not supported by the current technology. Even if an end-user can access a multiple set of resources, this requires significant technical expertise and understanding of low level details. End-users of distributed computing infrastructures want to concentrate on their research or business task, and do not want to become distributed computing experts.

Executing complex tasks on distributed computing infrastructures also requires tools for the composition and orchestration of simple jobs and services into more complex structures such as computational workflows. Grid workflow systems, for example Taverna (Oinn, T. et al. 2004), Triana (Churches, D. et al. 2006), Kepler (Jones, M. et al. 2006) or P-GRADE (Kacsuk P. & Sipos G. 2005), are widely utilised by e-scientists for job/service orchestration and execution. Executing a workflow that accesses multiple heterogeneous computational and data resources can be regarded as the most generic way of harnessing DCIs. The integration of the most commonly used job submission, service invocation and data access mechanisms into grid workflow solutions, and the ability of these workflow systems to share computation and data between each other would solve most of the interoperation challenges e-scientists face today. Moreover, integrating these workflow solutions into high level user interfaces and environments, such as grid portals or science gateways enable end-users to distance themselves from the complexity of the platform and concentrate on their research task instead.

The submitted work carried out by the candidate since 2005, provides a unique and comprehensive solution for the above described interoperability and accessibility problem at the level of computational workflows. The submission covers different aspects of workflow level interoperation and their integration into science gateways.

Interoperation at the level of workflows can be achieved inside one workflow or across several different workflow systems. Therefore, one can talk about intra- or inter- workflow interoperation, respectively (please see [12] for more details). In both cases two different aspects of interoperation need to be examined. The first aspect is the execution of workflow components on computing resources spanning several grids or DCIs. The second aspect is the movement of data between heterogeneous data resources and workflow components on different grids/DCIs. Table 1 (taken and adapted from [12]) summarises these areas.

Workflow level interoperation	WF component execution	Data resource access
Intra-workflow	Jobs or services of one particular workflow access heterogeneous computing resources from different Grids	Jobs or services of one particular workflow access heterogeneous data sources from different Grids
Inter-workflow	Jobs or services of multiple workflow systems access heterogeneous computing resources from different Grids	Jobs or services of multiple workflow systems access heterogeneous data sources from different Grids, (Data conversion between WF systems may be required)

Table 1 – Workflow level interoperation aspects

The outline of the submission is illustrated in figure 1. The figure shows the major areas covered by the candidate's research, and also explains how the submitted papers (the grey boxes including the numbers and titles of the papers) relate to these topics. The workflow level interoperability and accessibility work (red) can be divided into three main aspects (green): intra-workflow interoperation (details in section 3.1 of this commentary), inter-workflow interoperation (section 3.2), and application porting case-studies and methodologies for porting and deploying applications on interoperable grid infrastructures (section 3.3).

The largest part of the submission concentrates on intra-workflow interoperation aspects. Intra-workflow interoperation is considered both at workflow component execution and at grid data resource access levels. The major contributions in this part include the specification of a production quality legacy code deployment and submission service that allows the seamless integration of legacy applications into multi-grid workflows [1,2,3,4], the execution of Grid jobs and services on multiple Grid systems based on different Grid middleware [5,6,7], and the integration of heterogeneous data resources into these multi-grid workflows [8,9,10,11,12,13].

Inter-workflow interoperation is represented with one paper [14] presenting a unique solution for embedding non-native workflows into a hosting meta-workflow.

Finally, the candidate presents several application domain specific case studies [15,16,17,18], and introduces a generic methodology supporting the porting of applications to interoperable grid infrastructures [19,20]. The case studies illustrate the usability of the legacy code deployment and multi-grid job-submission and data access mechanisms by grid enabling applications using the unique methodology developed by the candidate.

The major contributions of the presented work, further analysed in the remaining part of this commentary, are as follows:

1. A production quality legacy code deployment and submission service that allows the seamless integration of legacy applications into multi-grid workflows.
2. A novel framework for executing legacy and non-legacy components of a workflow on multiple heterogeneous production grids.
3. A novel and generic framework for utilising heterogeneous grid file and data resources in multi-grid workflows.
4. A generic framework for embedding non-native workflows into a hosting meta-workflow.
5. A unique application development methodology and application support framework to facilitate the porting of applications to

interoperable distributed computing infrastructures.

The above referenced twenty publications were selected for this submission based on their relevance for the topic, their scientific merit, and the level of the candidate's contribution to the work. The candidate is the first author in fourteen of these publications, and also provided major contribution to the other papers, as it will be explained in this commentary. Table 2 relates the submitted twenty papers to specific sections of the submission explaining the contribution of each paper.

The overall research output of the candidate in the area directly related to this submission includes over 60 refereed journal papers, book chapters and papers in workshop and conference proceedings, as it is detailed in Annex 2. The candidate is also the co-owner of a US patent (Winter, S. C. et al. 2006), and his contribution to the area has been recognised by invitations to programme committees of several international conferences and workshops.

In the rest of this commentary the references are divided into two different categories. Referencing related research by other authors uses the Harward referencing technique, as it was used during this introduction. However, when referring to and explaining the contribution of papers from the submitted list of publications, the numbers identifying these papers are cited.

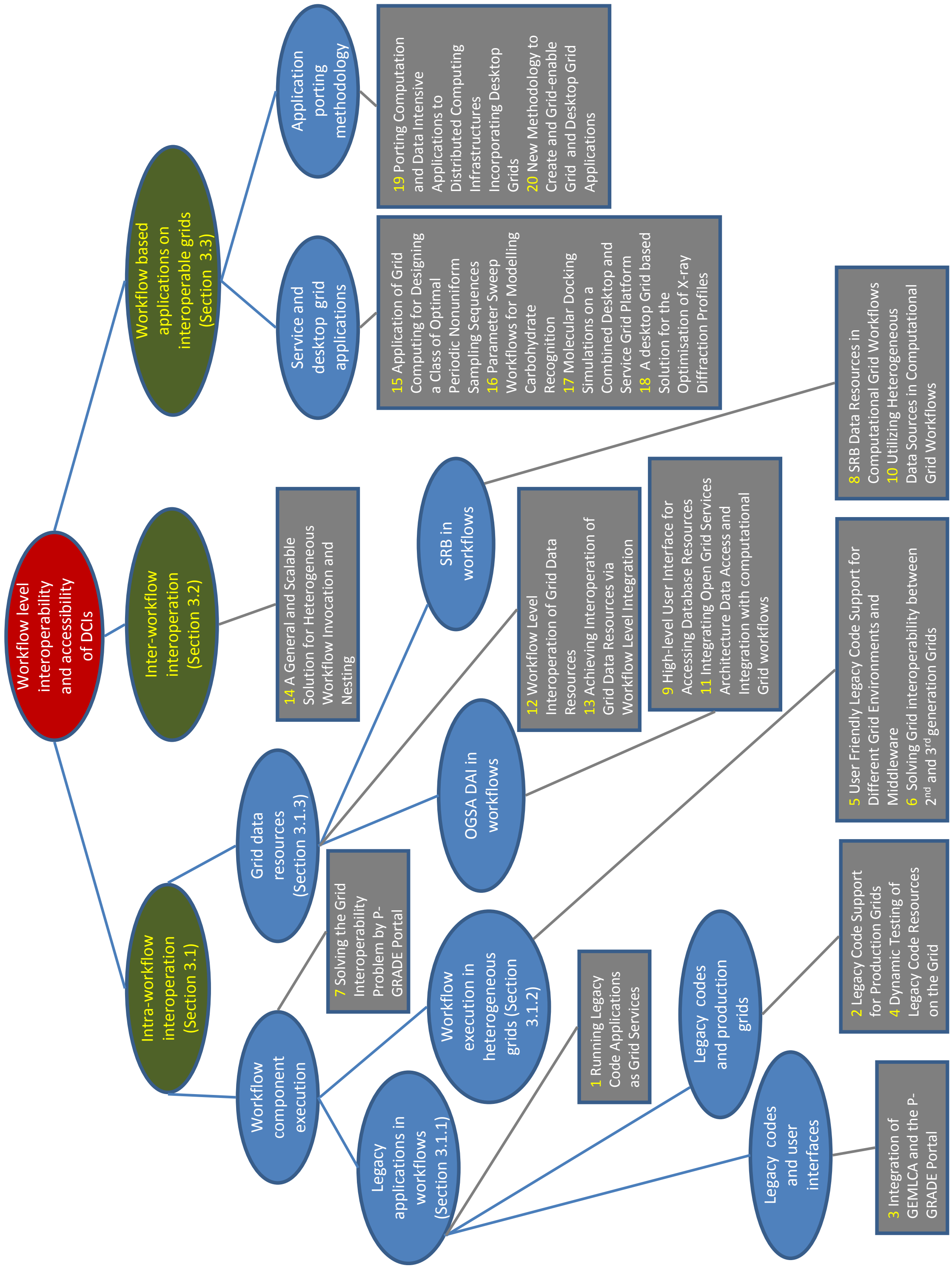

Figure 1 – Structural overview of the submission

Paper number	Title of paper	Section	Page number
1	GEMLCA: *Running Legacy Code Applications as Grid Services*	3.1.1	17
2	*Legacy Code Support for Production Grids*	3.1.1	17
3	*Integration of GEMLCA and the P-GRADE Portal*	3.1.1	18
4	*Dynamic Testing of Legacy Code Resources on the Grid*	3.1.1	18
5	*User Friendly Legacy Code Support for Different Grid Environments and Middleware*	3.1.2	19
6	*Solving Grid interoperability between 2nd and 3rd generation Grids by the integrated P-GRADE/GEMLCA portal*	3.1.2	19
7	*Solving the Grid Interoperability Problem by P-GRADE Portal at Workflow Level*	3.1.2	19
8	*SRB Data Resources in Computational Grid Workflows*	3.1.3	21
9	*High-level User Interface for Accessing Database Resources on the Grid*	3.1.3	21-22
10	*Utilizing Heterogeneous Data Sources in Computational Grid Workflows*	3.1.3	21
11	Integrating Open Grid Services Architecture Data Access and Integration with computational Grid workflows	3.1.3	22
12	*Workflow Level Interoperation of Grid Data Resources*	3.1.3	20
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17	Molecular Docking Simulations on a Combined Desktop and Service Grid Infrastructure	3.3	25
18	A desktop Grid based Solution for the Optimisation of X-ray Diffraction Profiles	3.3	25
19	Porting Computation and Data Intensive Applications to Distributed Computing Infrastructures Incorporating Desktop Grids	3.3	25
20	New Methodology to Create and Grid-enable Grid and Desktop Grid Applications	3.3	23

Table 2 –Summary of papers comprising the submission

2. Interoperability of Distributed Computing Infrastructures

The topic covered by the candidate's research in this submission is the interoperability of distributed computing infrastructures. Related research and the positioning of the candidate's work to this research are detailed in the individual publications. However, a short overview is given here summarising related research in areas covered by the candidate's work, and explaining the motivations behind approaching interoperability at the level of workflows when compared to middleware level.

The major force behind grid interoperation and interoperability research in the last five years has been the Grid Interoperability Now (GIN) community group of the Open Grid Forum (OGF), and its successor the Production Grid Infrastructures (PGI) working group. The GIN carried out several demonstrations and investigated the interoperation of middleware solutions in its four identified areas: information services, job submission, data movement, and authorisation and identity management (Riedel M. 2007/1, Riedel M. 2007/2). The PGI has continued this work and recently published a draft document on the production use cases of planned open standard specifications for production grid infrastructures (Riedel M. and Watzl J. 2011).

In conjunction with GIN and PGI activities, several research projects have also been investigating the middleware level interoperation of production grids. These efforts included work carried out by the OMII-UK (Open Middleware and Infrastructure Institute) team (Boardman R. et al 2007), and research conducted within the framework of the European CoreGrid project (Kertesz A. et al 2007), for example. Specific European projects, such as the GRIP (GRid Interoperability Project) project, or more recently the OMII Europe project have also been launched to solve long term interoperability between the most widely used Grid middleware solutions, including Globus (Foster, I. 2006) , gLite (Laure, E. et al. 2006) and Unicore (Nicole, D. A.

2005). More details on the state of the art of these research activities can be found in [12] and [13].

While all above projects concentrate on making cluster or supercomputer based service grid systems interoperable, the European EDGeS (Enabling Desktop Grids for e-Science, project number: RI 211727) and its follow-up the EDGI (European Desktop Grid Initiative, project number: RI 261556) projects created a bidirectional bridging mechanism (Urbah E. et al. 2009) between cluster based service grid, and BOINC (Anderson, D. P. 2004) and XtremWeb (Fedak G. et al 2001) based desktop grid systems.

Work is also ongoing making grids and clouds connected and interoperable with each other (e.g. Kacsuk P. et al 2010). The EDGI project, for example, uses cloud based worker nodes to enhance the performance of desktop grid systems and to provide required quality of service guarantees (Delamare et al 2011).

Different types of distributed computing infrastructures and projects/groups that are dealing with their interoperability are illustrated on Figure 2. Please note that the figure is for illustration only and does not intend to capture all interoperability related research. However, the figure shows the most important areas and activities which are related to the candidate’s work, and where concrete contribution has been made by the candidate. As shown in the figure, the main force regarding interoperability between different types of supercomputer and cluster based service grids is the PGI (GIN), while the desktop related activities and their connection to clouds are covered by the EDGI (and EDGeS) project (with significant contributions from the candidate, as detailed later).

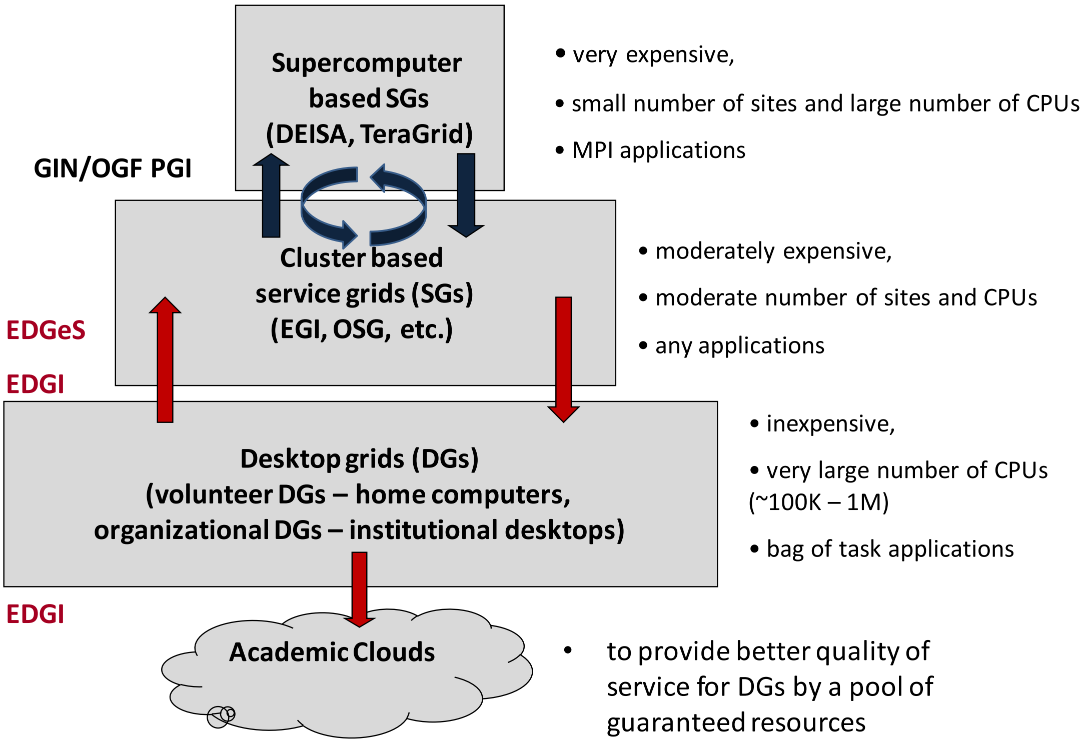

Figure 2 – Distributed computing infrastructures and major efforts to make them interoperable

The above described solutions aim to provide interoperability at the level of grid middleware by developing standards and standard based solutions, and directly integrating them into the grid middleware. Although middleware level interoperation is the foundation, end-users typically require high level tools to interact with resources. Also, middleware level interoperability typically requires standardisation. Unfortunately, standardisation and the widespread utilisation of these standards is a long and painstaking process where success is not always guaranteed. End-users want to utilise multiple production grids and heterogeneous resources here and now. They do not want to wait for the standardised grids and clouds where all this happens by default, as it may never come. What they need are solutions that make current tools and technologies all work together.

Workflow systems are widely utilised by end-users to provide a higher level abstraction of the underlying middleware and to allow executing complex tasks in an automated way. Enabling these workflow systems to utilise multiple grid middleware solutions and to work together seamlessly, provides an immediately usable solution for the interoperability problem. The aim of the presented research was to define different aspects of workflow level grid interoperation and provide ready to use interoperable solutions for end-users, by building on the GIN and PGI activities and also by extending them.

Despite the widespread utilisation of grid workflow engines, relatively small effort has been put into workflow level interoperation prior to the presented work. Grid workflow solutions are usually coupled with one particular grid technology and come with a custom user interface that does not integrate well into Web-based grid portals. The different workflow solutions use different workflow languages for representation and cannot share components or data with each other. Partially based on the results of this presented work, the European Commission has recently funded the SHIWA project (Sharing Interoperable Workflows for large scale scientific simulations on Available DCIs, project number: RI 261585) that is the first large project to be dedicated to the further research and exploitation of this area.

3. Contribution of the Presented Work

This section describes the contribution of the presented work in three areas related to the workflow level interoperability and accessibility of distributed computing infrastructures (see Figure 1 in Section 1). In each area the most important results enhancing the state of the art by the candidate are highlighted. Details of these results can be found in the related and referenced publications.

3.1 Intra-workflow interoperation

Grid interoperation at the level of workflows can be achieved inside one workflow (intra-workflow interoperation), or within several different workflow systems (inter-workflow interoperation). The majority of the candidate's presented publications are related to intra-workflow interoperation. The intra-workflow interoperation work concentrated on three main challenges, resulting in three major contributions:

- a production quality legacy code deployment and submission service that allows the seamless integration of legacy applications into multi-grid workflows,
- workflow based execution of grid jobs and services on multiple Grid systems based on heterogeneous grid middleware,
- and integration of heterogeneous data resources into these multi-grid workflows.

3.1.1 Production Quality Legacy Code Deployment and Submission Service

A very important aspect of intra-workflow interoperation is the ability to utilise legacy applications as components of computational workflows and to execute these legacy applications in multiple production grid systems. Legacy code applications can be described as codes from the past that are maintained because they work, often supporting mission critical functionalities. These applications are typically not grid enabled, and definitely not capable to run by default in multiple heterogeneous grid systems. The source code of these applications is either not available, or even if it is available it may take significant effort and require specific expertise to reengineer it.

The candidate is one of the architects and co-owner of a US patent (Winter, S. C. et al. 2006) regarding GEMLCA, Grid Execution Management for Legacy Code Applications. GEMLCA enables the publication and execution of legacy applications using a Grid service interface, without modifying or requiring access to the legacy source code. Compared to related solutions (Balis B. et al. 2005, Glatard T et al.2006, or Huang Y. et al 2003), GEMLCA represents a generic and non-invasive solution that allows the deployment of legacy applications as grid services by defining an XML-based Legacy Code Interface Description (LCID) file.

The candidate has worked as part of a team of six people designing and shaping the GEMLCA architecture, and contributed approximately 20% to the overall concept. The most comprehensive description of GEMLCA can be found in [1]. The paper was almost entirely written and edited by the candidate. The candidate’s contribution to the paper includes the definition and refinement of the GEMLCA concept, positioning the solution to related works and approaches, defining the integration of the solution with a high level portal interface, and designing the application scenario for providing proof-of-concept. The paper has been cited 95 times, according to Google Scholar.

Production grid infrastructures and their users demand specific characteristics from services that are deployed on the resources. Grid operators are typically reluctant to deploy and maintain new services on core nodes of the grid. However, providing these services in a 3rd party service provisioning model is typically accepted, supposing that the service is fully monitored and its state information is continuously available for both grid operators and end-users. In order to facilitate the wider take-up of a new value added service, such as the GEMLCA legacy code deployment and submission service, it is also necessary to provide a high level and easily accessible user interface to interact with the application.

The candidate was the major architect behind transforming GEMLCA into a production level service supporting users of the UK National Grid Service (NGS). This work has concentrated on three different aspects: a third party service provisioning model (1), the monitoring of GEMLCA resources (2), and integrating both the GEMLCA service and the monitoring tool into a grid portal environment (3).

Addressing the first challenge, the candidate has designed different models and proposed solutions for connecting a third party service such as GEMLCA to production grids. These solutions, described in detail in [2], address the issue of different grid middleware generations and service provisioning models. GEMLCA itself is a Web Services Resource Framework (WSRF) (Globus 2004) compliant grid service which was originally designed to call services deployed on grids based on 3rd generation grid middleware, such as Globus Toolkit version 4 (GT4) (Foster I. 2006). However, production grids at that time were typically operated on 2nd generation grid middleware (such as Globus Toolkit version 2).

The designed models have been implemented and incorporated into the current GEMLCA architecture. The first model stores the legacy codes in a central third party repository and submits them using common job submission mechanisms to the target production grid. This solution is suggested when the legacy application is simple and requires no additional deployment on the target resource. The second model is for more complex applications that require pre-deployment on the resources. These pre-deployed applications are then invoked by the GEMLCA service. While the first model was widely used in the first few years of operation, the second model also became more and more viable as the NGS started to pre-deploy the most widely used complex application packages on its resources (e.g. molecular dynamics applications, such as Gromacs (Lindahl E. et al. 2001) or Amber (Case D. A . et al. 2005).

The second challenge is to satisfy the service and resource monitoring requirements of production grids. Because of the transient nature of the grid, and because grid services, such as GEMLCA, typically rely on rather complex Grid middleware solutions, it is very important that both grid operators and end-users are aware of the failure of resources and could act accordingly. Providing this monitoring information is usually a pre-requisite before a service can be connected to a production infrastructure. To fulfil this requirement, GEMLCA has been extended with a monitoring tool, called GEMLCA Monitoring Toolkit (GMT), that reports automatically any failure to system administrators, and that also allows users to select only tested and working resources when mapping the execution of a legacy application.

The monitoring and resource availability framework was designed by the candidate and MSc student L. Bitonti working under his direct supervision. The solution is described in detail in [4]. The paper also illustrates how the architecture can be extended in order to enhance the capabilities of production grid systems and grid brokers with resource availability information and future prediction.

Finally, addressing the user friendly accessibility of legacy code submission and invocation, both the GEMLCA service and the monitoring toolkit have been integrated to the P-GRADE grid portal and workflow management environment.

The integrated solution enables e-scientists to map P-GRADE workflow components into legacy applications deployed in the GEMLCA legacy code repository, and also use the submission interface of GEMLCA to execute these workflows on second or third generation production grid resources. The portal has also been extended with a GEMLCA Administration Portlet that hides the syntax and structure of the Legacy Code Interface Definition file, and makes legacy code deployment easier. The integration of GEMLCA to the P-GRADE Grid portal is detailed in [3]. The candidate is the major architect behind this work while the implementation was carried out by the co-authors under the joint supervision of the candidate.

The integration of the GMT to the P-GRADE/GEMLCA environment is described in [4]. Site administrators can configure the GMT to run various probes at predefined intervals. The results are collected by a portlet that is integrated into the P-GRADE portal.

Based on the results of the above described papers, a production GEMLCA service front-ended by the P-GRADE portal has been set up in 2005 for NGS users. This service has been operational, with regular upgrades since that date. GEMLCA has also been applied by several European projects. For example, the EDGeS project utilised GEMLCA as its application repository (Urbah E. et al. 2009), while the coarse grained workflow interoperability solution of the SHIWA project is also GEMLCA based.

3.1.2 Workflow based Execution of Grid Jobs and Services on Multiple Grid Systems

The second major contribution in the area of intra–workflow interoperation is regarding the workflow based execution of grid jobs and services on multiple grid systems based on heterogeneous grid middleware.

Intra-workflow interoperation of workflow component execution was defined by the candidate in [12] as jobs or services of the same workflow that can be mapped to different production grids based on different grid middleware solutions. This interoperation allows end-users to utilise multiple production grids at the same time, significantly extending the pool of available resources. The candidate has designed and carried out the first workflow-level grid interoperability experiments where different submission mechanisms, grid middleware solutions and administrative domains have been applied within the same workflow.

The Grid community has devoted quite a lot of effort towards grid interoperability research. However, most of these efforts concentrated at middleware level solutions where the introduction of widely accepted standards was required. As accepting and adopting standards takes a long time, it left the grid user community with non-interoperable solutions in the meantime. The work of the candidate demonstrated that interoperability can be handled at a much higher level, the level of workflows, more efficiently and quickly. These solutions can also be embedded into grid portals and science gateways providing immediately usable solutions for scientists.

The work presented in this section is a natural continuation of the legacy code deployment work, as it is detailed in [5]. The earlier work has been extended to execute legacy applications on multiple grid middleware, in different production grids and administrative domains, and combine them into one workflow. The solution presented in [5] enables legacy code applications to be executed on grid resources based on 2nd and 3rd generation grid middleware, and also outlines how the solution can be extended to desktop grid systems. Moreover, GEMLCA is applied as a legacy code repository for Grids based on 2nd generation grid middleware by extending the direct job submission with repository based submission.

Different scenarios for the interoperability of workflow component execution are introduced and analysed in [6]. These scenarios and the executed experiments demonstrated that the candidate's work has successfully resulted in the workflow level interoperation of widely used production grid systems at the level of workflow component execution. The paper describes unique solutions on adding GT4 resources to GT2 Grids, connecting different GT2 and GT4 Grids, and connecting LCG/g-Lite based Grids with Globus Grids. Job submission in all scenarios is supported either directly or by submitting pre-deployed applications from an application repository. An application case-study illustrates the usability of the above described principles. The designed and analysed scenarios and the application case-study all represent the work of the candidate.

Results of the intra-workflow interoperation of workflow component execution work are summarised in and further extended in [7]. The paper utilises the above mentioned scenarios and solutions, and extends them with new concepts regarding the P-GRADE Grid portal. The P-GRADE related work (Section 3) is the work of the co-authors, while the interoperability scenarios and the application case-study are the work of the candidate. The paper has been cited 37 times, according to Google Scholar.

The candidate's work on the above area resulted in setting up of the GIN Resource Testing Portal (as described in [7]) in 2006 that was the only available solution at that time to execute Grid jobs and services on resources coming from different production grid systems. Extended with the work described in [4], it has also provided a seamless framework for monitoring the availability of GIN resources.

3.1.3 Integration of Heterogeneous Data Resources into Multi-grid Workflows

The third major contribution in the area of intra–workflow interoperation is regarding the integration of heterogeneous data resources into multi-grid workflows. This work has resulted in generic architectures and solutions for the integration of heterogeneous data resources into grid workflows. The concepts have been implemented within the P-GRADE portal and its workflow system. The enhanced P-GRADE grid portal that enables access to a wide range of grid file systems and database solutions have been deployed at production level as the NGS P-GRADE portal.

The candidate has defined the generic requirements towards intra-workflow interoperation of grid data resources in [12]. According to this definition, in a generic intra-workflow interoperation scenario the input files of the workflow can come from file systems, such as SRM (Sim A. et al. 2007) or SRB (Rajasekar A. et. al. 2003), or from database management systems, and the results can also be fed into any of these solutions. Both the file systems and the databases can be located in different production grids, and the jobs of the workflow can also be mapped to different grids (if we desire intra-workflow interoperation at workflow component execution level too).

None of the grid workflow systems prior to the candidate's research supported the above model. In order to provide a generic interoperable solution for data access at the level of workflows, the integration of widely used file and database access mechanisms into existing workflow systems was required.

The generic requirements towards this interoperation, and the categorisation and analysis of the different aspects and scenarios have been introduced in [12]. This publication is the candidates own work with support and guidance only from the PhD supervisory team. The publication identifies areas and key technologies for solving the intra-workflow interoperation of grid data resources. Based on these identified areas, the candidate's research has concentrated on feeding data stored in file systems and relational and xml based databases into workflows. The achieved interoperation is based on the integration of two widely used technologies, namely the Storage Resource Broker (SRB) (Rajasekar A. et al. 2003) and the Open Grid Services Architecture Data Access and Integration service (OGSA-DAI) (Antonioletti M. et al 2005), into grid workflows systems. The justification of the selection of these technologies and their generic description can be found in respective publications (e.g. [12] and [13]). Besides the generic concepts, [12] also summarises the early results of the SRB and OGSA-DAI integration work that have been introduced and described in detail in other publications (SRB: [8] and [10], OGSA-DAI: [9] and [11]).

Integrating SRB data resources into computational Grid workflows is analysed in [8]. The candidate suggested and compared different ways of integration. The suggested solutions include indirect integration when data stored in SRB catalogues is handled by an auxiliary tool, e.g. a separate browser portlet, and direct integration when SRB is closely integrated with the workflow system.

The direct integration approach has been the focus of [8] describing how SRB input and output ports can be added to workflow solutions. The paper concentrates on three major aspects of the integration: the setting up and configuration of the SRB client environment (1), the definition of SRB ports in the workflow editor (2), and the transfer of data between the executor grid nodes and the SRB catalogues (3). This work has lead to the first data interoperation scenarios as introduced in [8]. The indirect integration via a separate SRB portlet extends the above work in [10].

The design and analysis of the integration concepts and scenarios are the work of the candidate. The implementation of the system has been carried out by Alexandru Tudose under the direct supervision of the candidate.

Parallel to the above work, the role and usability of database management systems in grid workflows has also been investigated. Although database integration to grid systems is addressed in several forums such as the DAIS

(Data Access and Integration Services) working group of the OGF or the OGSA-DAI project (Antonioletti M. et al 2005), interoperation of file storage solutions and databases has not been included even in the GIN and PGI activities. While direct data transfer would be rather difficult between these logically different solutions, it is possible to combine file and database resources at workflow level.

Although the DAIS Working Group is working on the specification of a generic interface to expose database operations, there is also a clear need for higher level services abstracting database access and making application development easier. A generic tool that exposes database operations as services is OGSA-DAI. OGSA-DAI has been selected by the candidate as the middleware level solution to be integrated with workflow solutions due to its flexible architecture and widespread utilisation by the Grid community (for more justification and related work please refer to [9] and [11]). Similarly to the SRB related work, different options and scenarios have been investigated and implemented in case of OGSA-DAI.

As a result of this work the first comprehensive set of end-user interfaces, a set of portlets that provide rich and high-level functionality to access generic OGSA-DAI services, have been designed and developed [9]. This set of portlets provides a wide range of functionality for managing and utilising databases exposed with OGSA-DAI, and represent a significant advance when compared to related earlier solutions (see [9] for details). The designed and implemented functionalities can be divided into four major components implemented as four separate portlets:

- Managing data services where existing services can be listed with their relevant properties, services can be removed and new services can be added.
- A database browser interface where users can explore the content of available services and resources.
- Executing advanced queries allowing data to be displayed on the screen or to be delivered to a set of files for further processing.
- Updating the content of a database through queries or by delivering

data from a set of files.

This work is a joint effort of the candidate and Tamas Kukla who worked as an MSc student under the direct supervision of the candidate.

Although the OGSA-DAI portlets, integrated to any JSR-168 (JSR 168 2003) compliant Grid portal enabled end-users to manipulate data from a high-level interface, the generic data interoperation scenario described earlier, desired a closer and more automated integration of OGSA-DAI and grid workflow systems.

The different aspects of integrating OGSA-DAI with grid workflow solutions have been analysed and critically evaluated in [11]. Five different aspects of this integration have been considered: data staging (1), subject of integration (2), request representation (3), support of functionality (4), and client location (5). Based on the analysis of the above aspects, a generic integration approach has been proposed and implemented based on the GEMLCA legacy code repository and submitter solution (see earlier work of the candidate as summarised in [1]). The solution enables OGSA-DAI clients, accessing remote OGSA-DAI services, to be deployed as GEMLCA legacy codes. These GEMLCA jobs can be embedded into complex P-GRADE portal workflows as components.

The achieved results in the area of intra-workflow interoperation of grid data resources have been consolidated and summarised in [13]. As a result of this work a generic solution to address the data interoperation scenario first introduced in [12] has been proposed. A reference implementation based on the P-GRADE portal and workflow system has been successfully created, and its applicability has been illustrated in two different case studies (traffic simulation and hospital profiling, as described in [13]). The presented work is the result of the candidate’s own research, while the OGSA-DAI implementation was carried out by co-author Tamas Kukla.

3.2 Inter-workflow interoperation

In case of inter-workflow interoperation (as defined by the candidate in [12]) jobs or services of multiple workflow systems are accessing heterogeneous computing and data resources from different Grids. Work on the interoperation of multiple heterogeneous workflow systems was initiated by the candidate and work presented in [14] is the joint effort of the candidate and Tamas Kukla. (This work has been further carried on and became the basis of the PhD thesis of Tamas Kukla in which the candidate had only consulting role.)

A general and scalable solution for heterogeneous workflow invocation and nesting based on the GEMLCA service is presented in [14]. The designed and implemented system represents a generic and unique solution how non-native workflows can be embedded into a native meta-workflow. The non-native workflow embedded into the meta-workflow is represented as a GEMLCA job. The workflow engine of the non-native workflow component is described as a GEMLCA legacy code and published in the GEMLCA legacy code repository. The meta-workflow developer can select the target workflow engine description from the GEMLCA repository, and pass the executable non-native workflow to the engine as input parameter.

The above concept has been implemented inside the P-GRADE grid portal and workflow environment and allows Taverna, Triana and Kepler non-native workflows to be embedded into P-GRADE portal meta-workflows. The solution has been deployed within the NGS P-GRADE portal and accessible at production level for UK users. The European SHIWA project has also utilised this concept as its starting point for realising coarse-grained workflow interoperability inside the SHIWA Simulation Platform.

3.3 Methodology and Case-studies

The success of any principle and solution can only be measured by its real usability for end-user scenarios. The interoperation principles and solutions designed by the candidate and described earlier have been prototyped and evaluated in multiple user scenarios in different scientific domains and disciplines. Besides prototyping the interoperability solutions, the candidate has also actively worked on and provided significant contributions to developing new methodologies for application porting and supporting user communities. Papers presented in this section describe the results of these application porting activities. Please note that only a subset of all results have been published until the day of submission of this PhD thesis. Full list of application support activities that are lead and co-ordinated by the candidate are available on the W-GRASS Website (http://wgrass.wmin.ac.uk).

As major contribution to the above area, the candidate has developed a unique methodology (EDGeS Application Development Methodology – EADM) [20] to port applications to interoperable service and desktop grid infrastructures. EADM is the first formal methodology specifically addressing requirements and problems to be considered when developing or porting applications to interoperable service and desktop grid infrastructures. The methodology is based on the generic systems development life-cycle. The uniqueness is provided by defining deliverable templates and specifying aspects of the development process that must be considered when targeting a combined service and desktop grid platform. The candidate is the author responsible for the development of the methodology, while the co-authors contributed the technical descriptions of the tools supporting EADM in the annex of the paper [20].

The candidate has also been the co-founder and leader of the Westminster Grid Application Support Service (W-GRASS), and has been leading and co-ordinating application porting activities in several European projects (EDGeS, EDGI and DEGISCO). As a result of these activities over thirty scientific applications have been grid enabled and successfully applied by end-user communities (details of some of these applications are described in papers [15,16,17,18]). These applications utilise the interoperable solutions designed by the candidate and the majority of them have been ported following the EADM methodology. EADM has also been successfully applied by several external application development centres (e.g. CNRS France, G.V.Kurdyumov Institute for Metal Physics of the Ukrainian National Academy of Sciences, Huazhong University Of Science and Technology China, SZTAKI Research Institute Hungary, Universidade Federal de Campina Grande Brazil, Institute for Systems Analysis of Russian Academy of Sciences, Kazakh-British Technical University Kazakhstan, Cardiff University, Academia Sinica Taiwan).

The grid based implementation of a digital signal processing (DSP) application to design a class of optimal periodic non-uniform sampling sequences has been described in [15]. The application has been migrated to both service and desktop grid infrastructures, and the efficiency and usability of both solutions have been analysed and compared. The service grid solution utilises GEMLCA and the P-GRADE grid portal, and enables the creation and execution of P-GRADE workflows composing of GEMLCA jobs in heterogeneous grid infrastructures based on multiple middleware. The desktop grid solution is based on the SZTAKI Desktop Grid (Balaton Z. et al. 2007) technology, a modified version of BOINC (Anderson, D. P. 2004). The comparison of the solutions was based on deployments on the local University of Westminster computing clusters (as parts of the UK NGS), and a local desktop grid installation spanning several teaching laboratories at UoW. The application case study illustrated how the GEMLCA extended P-GRADE portal could be utilised in complex application scenarios to harness the largest number of available resources for end-users. The concept of the Grid based solutions and their comparative analysis are fully the work of the candidate.

Although the service and desktop grid based solutions were completely independent and non-interoperable at the time of writing the above paper, later this application has also become the first case study to test and evaluate the bi-directional bridging mechanism developed by the EDGeS project connecting service and desktop grid infrastructures. As a result of that work the DSP application could run on combined service and desktop grid infrastructures utilising both platforms within one experiment.

The design and implementation of a parameter sweep workflow for modelling carbohydrate recognition is the subject of [16]. The latest version of the P-GRADE Grid portal family, the WS P-GRADE portal (Kacsuk P. et al 2008) has been utilised to build a complex workflow to model receptor/ligand interaction. The workflow has standard P-GRADE and GEMLCA jobs, and users can map these jobs to different production grids based on heterogeneous middleware. The workflow combines several widely utilised bio-molecular application packages, for example the Gromacs (Lindahl E, et al, 2001) and AutoDock (Morris G. M., et al. 1998) program suites, and enables the automated execution of complex user scenarios. The concept and design of the workflow is the work of the candidate, while the implementation and the domain specific expertise are coming from the co-authors.

Applications ported to combined and interoperable service and desktop grid infrastructures are presented in [17] and [18]. These application examples utilise the EDGeS Application Development Methodology (EADM) for the porting. The EADM, presented in detail in [20], has been fully developed by the candidate. The methodology provides a generic framework and documentation template for porting applications to combined service and desktop grid infrastructures. The EADM defines stages and actors responsible for these stages. It also lists aspects and representative problems and questions that need to be addressed at each stage. The methodology has been utilised to port over thirty applications to grid infrastructures within the framework of the EDGeS, EDGI and DEGISCO European projects. Representative examples for these applications where the porting has been designed and supervised by the candidate are described in [17] and [18].

A continuation of the bio-molecular simulation work of [16] is presented in [17]. The paper in [17] utilises the user scenario described in [16], and proposes, designs, implements and evaluates solutions for bridged service and desktop grid infrastructures. The Autodock based docking phase of the workflow described in [16] has been ported to BOINC based desktop grid infrastructures utilising the EADM methodology. The application is executed in three different scenarios providing different user interface and entry point for biologist researchers (a BOINC master application, a WS P-GRADE based graphical user interface, and a g-Lite command line interface).

Application porting activity using the EADM methodology but representing a completely different application domain is described in [18]. The paper presents the porting of an application designed to optimise x-ray diffraction profiles on a combined service and desktop grid infrastructure. The work has been carried out in collaboration with researchers from the University of Extremadura in Spain. The ported application has been running at production level on the resources of the University of Westminster local desktop grid and the EGEE grid via the EDGeS bridging mechanism.

Experiences with application porting using EADM to combined service and desktop grid platforms are summarised in [19]. This paper builds on the experiences gained from the EDGeS, EDGI and DEGISCO projects, and describes the generic and application scenario specific requirements when porting applications to the combined grid. The paper is fully based on the candidate’s work with the exception of the data intensive application scenarios (work carried out by co-author Ian Kelley).

4. Summary of contributions

As grid and other distributed computing infrastructures evolve, and as their take up by user communities is growing, the importance of making different types of DCIs based on a heterogeneous set of middleware interoperable is becoming crucial. This PhD submission presents a unique solution to the challenge of the seamless interoperation of distributed computing infrastructures at the level of workflows. The invented and developed framework enables the execution of legacy applications and grid jobs on multiple grid systems, and the feeding of data from heterogeneous file and data storage solutions to these workflow components. Moreover, the solution provides a high level user interface that enables e-scientist end-users to conveniently access the interoperable grid solutions without requiring them to study or understand the technical details of the underlying infrastructure. Besides the technical framework, the candidate has also developed an application porting methodology that enables the systematic porting of applications to interoperable and interconnected grid infrastructures, and facilitates the exploitation of the technical framework.

The major contributions by the candidate summarised in this commentary and described in detail in the papers can be divided into three main categories. Contributions 1, 2 and 3 refer to intra-workflow interoperation. Contribution 4 is related to inter-workflow interoperation, while contribution 5 is in the area of application development and support methodologies. The contributions are the following:

1. *A production quality legacy code deployment and submission service that allows the seamless integration of legacy applications into multi-grid workflows.* The candidate has significantly contributed to the architecture of the GEMLCA legacy code deployment framework, and was the major architect for defining the requirements and designing the necessary solutions in order to transform GEMLCA into a production level service. This work included the design of different models for connecting third party services to production grids, the creation of a

resource monitoring framework for monitoring legacy code resources, and the concepts of integrating legacy applications into portals and workflows.

2. *A novel framework for executing legacy and non-legacy components of a workflow on multiple heterogeneous production grids*. The solution enables intra-workflow interoperation of workflow component execution when jobs or services of the same workflow can be mapped to different production grids based on different grid middleware solutions. This functionality allows end-users to utilise multiple production grids inside one workflow significantly increasing the amount of available resources.
3. *A novel and generic framework for utilising heterogeneous grid file and data resources in multi-grid workflows.* The solution enables intra-workflow interoperation of grid data resources where jobs or services of one particular workflow access heterogeneous data resources from different grids. The candidate has analysed alternatives, and designed and prototyped unique and generic solutions for the integration of grid based file and database management solutions to computational workflows.
4. *A generic framework for embedding non-native workflows into a hosting meta-workflow.* The candidate has significantly contributed to the creation of a generic framework for heterogeneous workflow nesting and invocation that allows non-native workflows to be called and executed from a hosting meta-workflow. The solution provides coarse-grained workflow interoperability where sub-workflows can be reused as part of the embedding meta-workflow, and significantly reduces development time and effort by avoiding unnecessary duplication of work.
5. *A unique application development methodology and application support framework to facilitate the porting of applications to interoperable distributed computing infrastructures.* The candidate has developed an application porting methodology and support framework

to port applications to combined service and desktop grid infrastructures. The methodology provides the first comprehensive set of guidelines to support application porting to interoperable grid infrastructures in a formalised manner. The suitability of the methodology and the designed interoperable frameworks has been demonstrated via several case studies.

The presented research and the above described contributions represent a new approach towards grid interoperability when compared to middleware level solutions. The candidate's work presented general frameworks and reference implementations when solving the grid interoperability problem at workflow level. Based on the presented frameworks and principles interoperable solutions can be built quickly. However, as these solutions are currently built on top of non-interoperable grid middleware, they still require the lower level standardisation efforts.

The above described contributions and presented results have also facilitated further research in the areas of interoperability and application support that the candidate is currently involved in. The focus of the interoperable solutions has shifted from service grid infrastructures to incorporate additional DCIs such as desktop grid systems and clouds. In line with these activities the application support and porting also concentrates on these additional infrastructures. These activities are demonstrated by current research grants from European and UK funding bodies where desktop grid and cloud infrastructures are utilised (e.g. the candidate leads the work that prototypes the Autodock molecular docking suite on the European Venus C project's cloud based infrastructure, and has also contributed to the UK EPSRC/JISC funded Optimal Scheduling of Scientific Application Workflows for Cloud-augmented Grid Infrastructures project).

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Annex 1 – Full reference of submitted papers

Full reference of papers comprising the submission

LEGACY CODE DEPLOYMENT:

1. Thierry Delaittre, **Tamas Kiss**, Ariel Goyeneche, Gabor Terstyanszky, Stephen Winter, Peter Kacsuk: GEMLCA: *Running Legacy Code Applications as Grid Services*, **Journal of Grid Computing** Vol. 3. No. 1-2. June 2005, Springer Science + Business Media B.V., Formerly Kluwer Academic Publishers B.V. ISSN: 1570-7873 (Paper), pp 75-90, 1572-9814 (Online), http://dx.doi.org/10.1007/s10723-005-9002-8

2. **Tamas Kiss**, Gabor Terstyanszky, Gabor Kecskemeti, Szabolcs Illes, Thierry Delaittre, Stephen Winter, Peter Kacsuk, Gergely Sipos : *Legacy Code Support for Production Grids*, Conf. Proc. of the Grid 2005 - **6th IEEE/ACM International Workshop on Grid Computing** November 13-14, 2005, Seattle, Washington, USA, ISBN: 0-7803-9492-5, pp 278-283, http://delivery.acm.org/10.1145/1260000/1253508/01542754.pdf?ip=161.74.220.149&CFID=38456609&CFTOKEN=12216845&__acm__=1315300843_ae6e98dce25b220b20170698942ad581

3. **Tamas Kiss**, Gergely Sipos, Peter Kacsuk, Krisztian Karoczkai, Gabor Terstyanszky, Thierry Delaitre: *Integration of GEMLCA and the P-GRADE Portal*, Proceedings of Grid Systems, Tools and Environments, **CoreGrid WP7 Workshop as part of the Grids@Work Week**, Sophia Antipolis, France, October 12th, 2005. Editors: R. M. Badia, F. Baude, V. Getov, T. Kielmann, I. Taylor, CoreGrid TR-0043, pp 52-57, http://www.coregrid.net/mambo/images/stories/TechnicalReports/tr-0043.pdf

4. Luigi Bitonti, **Tamas Kiss**, Gabor Terstyanszky, Thierry Delaitre, Stephen Winter, Peter Kacsuk, *Dynamic Testing of Legacy Code Resources on the Grid*, Conf. proc. of the **ACM International Conference on Computing Frontiers**, Ischia, Italy May 2-5, 2006,

ISBN 1-59593-302-6, pp 261- 268,
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INTRA-WORKFLOW INTEROPERATION OF WORKFLOW COMPONENT EXECUTION

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