SIMDAT

Data Grids for Process and Product Development using Numerical Simulation and Knowledge Discovery

Project no.: 511438

Grid-based Systems for solving complex problems – IST Call 2

Integrated project

SIMDAT

Deliverable

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Table of contents

1 Introduction....6
2 Description of scenarios....7
2.1 Optimisation....7
2.2 Cost modelling....8
3 PM30 prototype....9
3.1 Overview....9
3.2 Developments....10
3.2.1 New Services....10
3.2.2 PSE Integration....11
3.2.3 Workflow Advisor....15
3.2.4 Cost Estimation....18
3.3 Deployment....19
3.4 Requirements status as of PM30....21
3.4.1 Grid Technology/Distributed Data Access....21
3.4.2 Administration of Virtual Organisation....22
3.4.3 Workflow....23
3.4.4 Analysis Services....24
3.4.5 Ontologies....25
3.4.6 Knowledge Services....26
3.5 Validation....27
3.6 Outstanding Issues....28
3.7 Summary....28
4 Description of the next prototypes (PM36 and PM42)....30
4.1 Product Knowledge....30
4.2 Process Knowledge....31
4.3 Validation and system metrics....32
5 Resulting requirements....33
6 Conclusion....42
7 References....43

Definitions, Acronyms and Abbreviations

Acronyms

PKI	Public Key Infrastructure
PSE	Problem Solving Environment
COTS	Commercial off the shelf
QoS	Quality of Service
CA	Certificate Authority
TLS	Transport Layer Security
RSM	Response Surface Modelling
SLA	Service Level Agreements
VO	Virtual Organisation

Executive Summary

This document discusses the aerospace activity prototype for the interoperability phase and describes the plans for the prototype for the knowledge phase of the project. The objective of the interoperability phase of the project was to demonstrate interoperability within the system. In order to demonstrate this, the connectivity phase prototype was extended with new services, workflow interoperability was demonstrated and the Grid middleware was integrated with several commercial problem solving environments. Highlights of the work carried out include:

- Extension the phase one scenario to include new services introducing new partners to the VO.
- Adoption GRIA 5.0.1
- Moved to new Business Cooperative VO model.
- Successfully demonstrated using SIMDAT technologies from within several commercial PSE.
- Successfully demonstrated interoperability of COTS PSE and other workflow tools.

A cost modelling scenario was developed and a prototype produced that demonstrated the use of semantic technology to quickly integrate data from multiple sources in the context of a cost estimation.

1 Introduction

This document is a report that describes the aerospace prototype implementation for the interoperability phase of the project as specified in SIMDAT Annex 1- “Description of Work” [1]. It uses the technologies outlined in D11.2.2 [2] and is designed to fulfil the scenarios described in D11.2.1 [3].

The primary focus of the aerospace activity is demonstrating how Grid technologies can be deployed to aid in complex collaborative engineering tasks. This is of particular interest to the aerospace industry as the majority of product development takes place in a collaborative fashion and these collaborations often cross organisation and international boundaries. The goal of this phase of the project was to demonstrate interoperability in the Grid system and produce a prototype showing this interoperability in action. This document describes the prototype produced for this phase and advances made up to project month 30 it also evaluates the requirements set out for this phase and validates them against progress made. It also looks ahead to the next phase and the planned prototype development and requirements.

2 Description of scenarios

This chapter contains a brief overview of the aerospace scenarios for further information about the scenarios please see D.11.2.1 [3]

2.1 Optimisation

The optimisation scenario is representative of a real world collaborative design problem. The scenario involves the optimisation of the wing of a BAE 146 Regional Aircraft. High lift devices result in increased noise and the aim is to reduce the extra noise generated by the wind during flap deployment without damaging its lift characteristics. As well as maintaining the required lift there are structural constraints to be taken into account. So this optimisation involves a number of different analysis that need to be tied together to solve one problem.

In the scenario BAE Systems are playing the part of a prime contractor who then subcontracts the optimisation to the University of Southampton (UoS) who perform the optimisation using analysis services from three external companies (in the scenario BAE, EADS and MSC). This involves a optimisation service at UoS driving the optimisation and coordinating the other services. The top level workflow for this scenario is shown below:

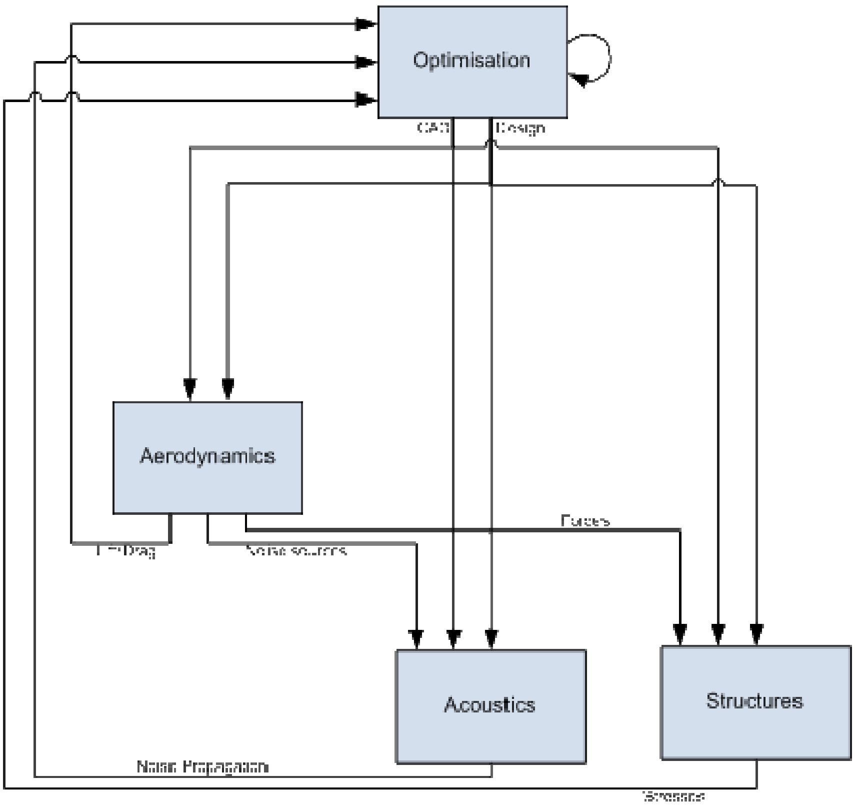
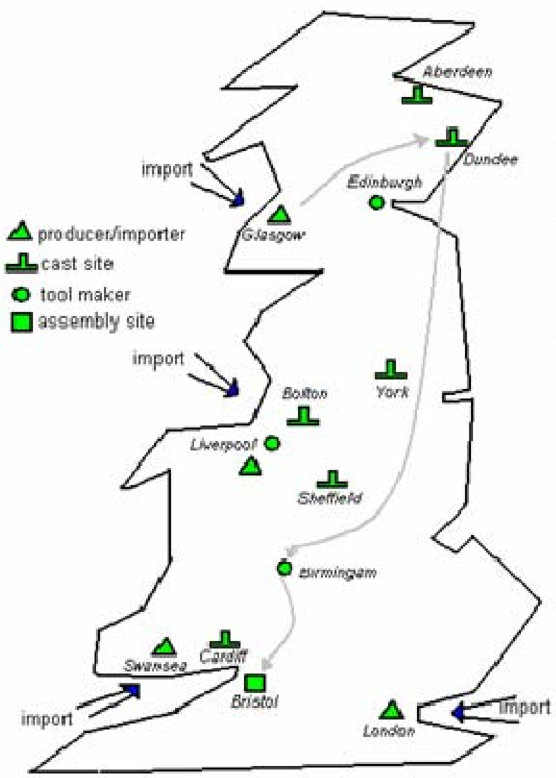


Figure 1 – Top Level Workflow

The system is built from a series of workflows, from this top level view to the individual analysis service workflows. As a different company is responsible for each workflow they might be using different workflow tools to publish these workflows. A key aim of the interoperability phase was to show how multiple workflow tools and PSE's could be used in such a system.

2.2 Cost modelling

The cost modelling scenario is a supplier integration problem where a manufacturer needs to be able to make reliable cost estimation on data coming from various sources. The sources may be a mixture of databases, flat files or spreadsheets and the user wants to be able to integrate the data into the cost estimation seamlessly. The data may also contain historical information that may allow data mining to predict trends and project future costs and the data mining algorithms should be able to run on the integrated data sources. The scenario is outlined below:



An assembly plant in Bristol needs to produce two units a month. A unit consists of 16 components. It takes 20 tonnes of Aluminium to produce 8 components. The component is manufactured by casting and tooling. The Bristol plant has associations with three tooling specialists: Liverpool, Birmingham and Edinburgh. Further the Bristol plant uses casting sites: Aberdeen, Bolton, Cardiff, Dundee, Sheffield or York. And its preferred importers are in: Glasgow, Liverpool, London and Swansea,

Contracts can be moved with one months notice between these sites

Figure 2 – Supplier integration scenario

3 PM30 prototype

3.1 Overview

The PM30 prototype was the prototype for the interoperability phase of the project and as such we aimed to demonstrate interoperability of the workflow and problem solving environments. This builds on the first prototype that demonstrated heterogeneous backend systems being accessed by a single client application through the GRIA job interface. With the PM30 prototype we were aiming to demonstrate heterogeneous front ends accessing the heterogeneous backend systems.

A prototype was produced for each of the scenarios described in section 4 and both prototypes were demonstrated at the 2nd annual review. Figure 3 shows the technologies from the SIMDAT portfolio that were used in the optimisation scenario prototype.

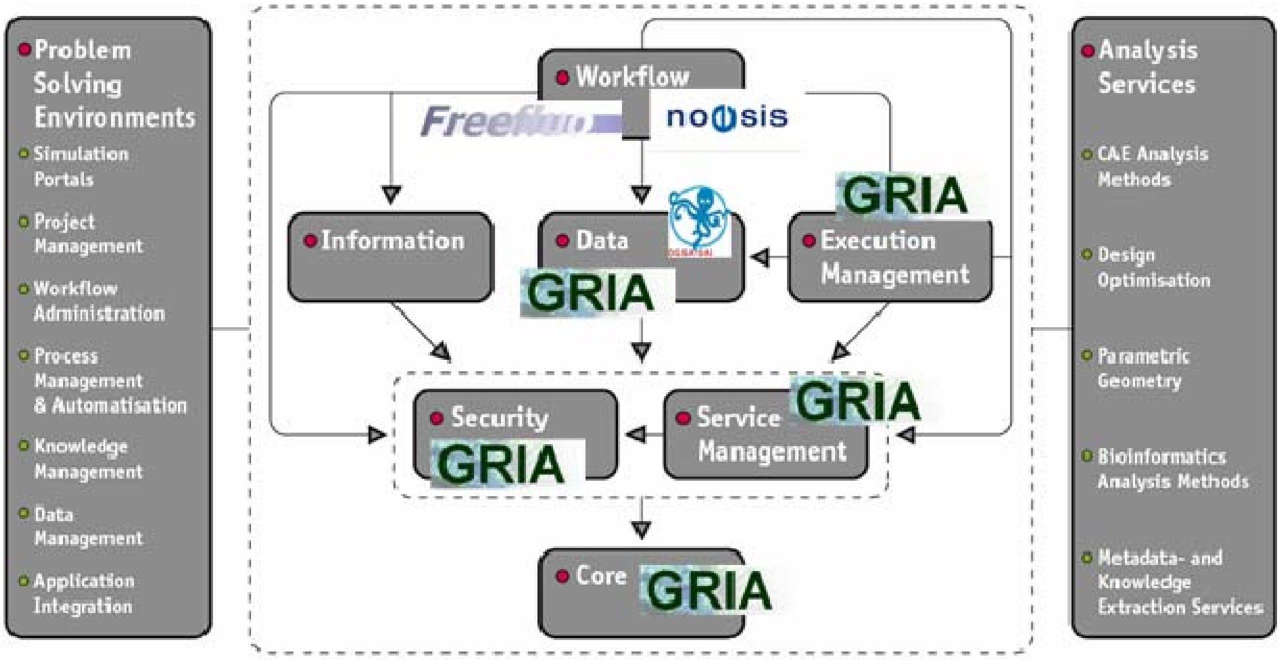


Figure 3 Aerospace SIMDAT Architecture Optimisation Scenario Usage

The prototype implementation is based on GRIA 5.01. GRIA provides the core job services, the ability to upload and download data to data stagers as well as providing the authorisation and authentication services. It is particularly suited to the aerospace applications due to the ease of wrapping legacy codes and interfacing with job schedulers. OGSA-DAI is accessible via a GRIA interface and is used for storing optimisation results. The workflow engines being used in the system include Freefluo and Optimus; both of these have been made accessible via the GRIA job interfaces and this gives us the ability to treat entire workflows as single GRIA accessible services. For the PM30 prototype new problem solving environments and analysis services were introduced.

Figure 4 shows the technologies used in the prototype implementing the cost estimation scenario. Ontoprises Ontobroker technology was used to do the semantic integration of the various data sources and this involved wrapping some of the data sources and making them available as OGSA-DAI databases.

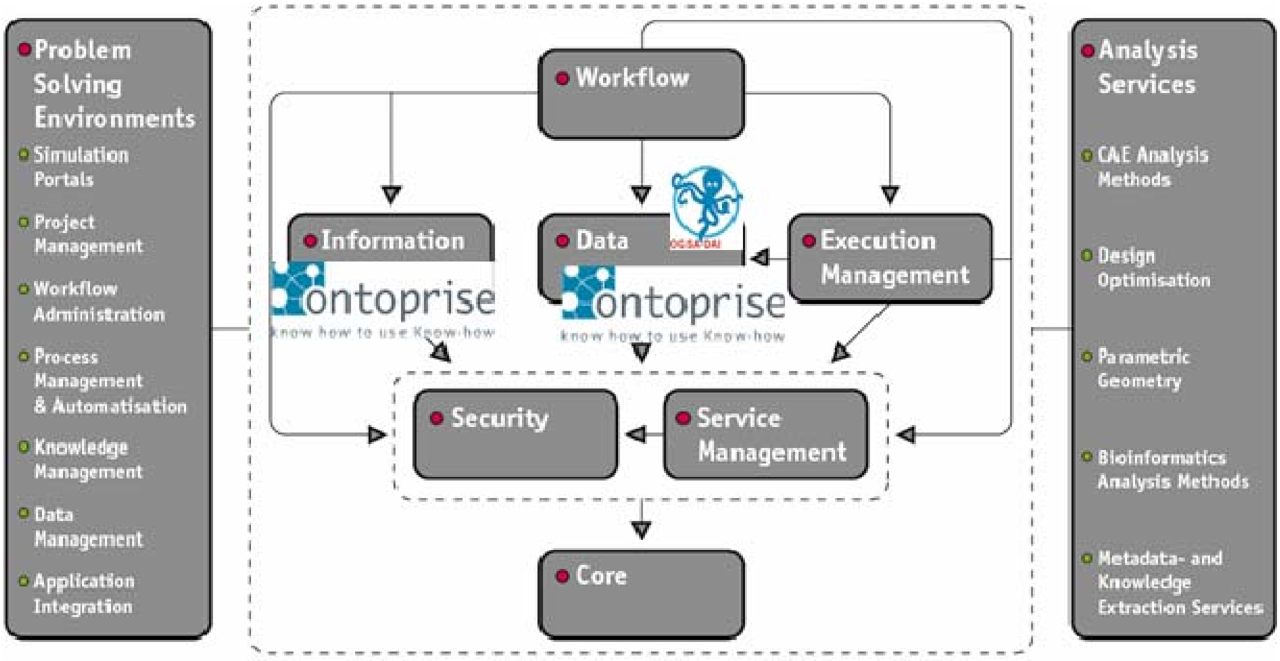


Figure 4 Aerospace SIMDAT Architecture Cost Estimation Scenario Usage

The two architecture diagrams show that between the two prototypes the aerospace activity uses technology from each area within the SIMDAT portfolio and that the portfolio matches all of our requirements.

3.2 Developments

Several of the major developments carried out for the PM30 prototypes are outlined below. The main focus of this prototype was to demonstrate interoperability.

3.2.1 New Services

The previous prototype has been extended with the addition of 3 new services. They are a structural analysis services, a response surface modelling service and a duplicate CATIA service.

The response surface modelling service was implemented by Noesis using thier Optimus package. It consists of three GRIA services – create RSM, evaluate RSM and run Optimus workflow. The services allow members of the VO to create an RSM using Optimus and then store that RSM as a data stager where it can be added to or used in an evaluation later. The RSM can also be downloaded and used locally. The ability to run Optimus workflows as a service means that a workflow constructed in Optimus can be called from any PSE that can call GRIA services, this is an example of workflow runtime interoperability described in D5.2.3 [4]

A new CATIA service has been deployed. Contrary to the one hosted by the University of Southampton, this one is deployed within a Windows Virtual Machine running on a VMware ESX Server. The backend used by GRIA is condor. Once the job is submitted, it is allocated to the only machine available in the pool. The CATIA part is transferred together with the command file. Then the job starts a cmd shell that calls CATIA in batch mode to generate the required geometries from the parameterised one.

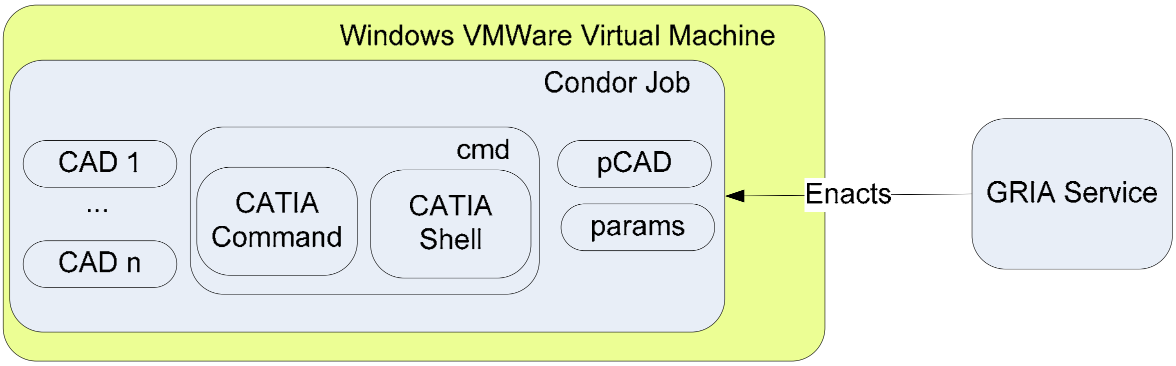


Figure 5: CATIA Service Architecture

The structural service was provided by MSC and is based on the reference implementation of an analysis service. The service was based on GRIA 5.01 and runs at MSC Munich. The service accepts an IGES geometry and performs the following steps:

- Generate a mesh using Patran;
- Assemble mesh and loadcase into a Nastran model;
- Use Nastran to do a simple stress analysis;
- Extract a key result (like maximum stress) and return the requested value.

The loadcase information comes from the service running at BAE and as well as receiving the geometry the structural service has a dependency on the aerodynamic services.

3.2.2 PSE Integration

3.2.2.1 ModelCenter

ModelCenter is a graphical problem solving environment from Phoenix Integration. It is used heavily in the aerospace industry for product optimisation and integration. BAE were interested in using ModelCenter to enact the SIMDAT workflows and so the integration with GRIA services was investigated. ModelCenter provides a Java interface for creating new analysis service components, using this and the GRIA 5 Java API BAE created three new plug-in components for ModelCenter. They are upload, download and job components. The job component lets the user select a GRIA server to query and retrieve the list of available job services; the user can then select the required service and the component will be added to the ModelCenter workflow with the correct inputs and outputs.

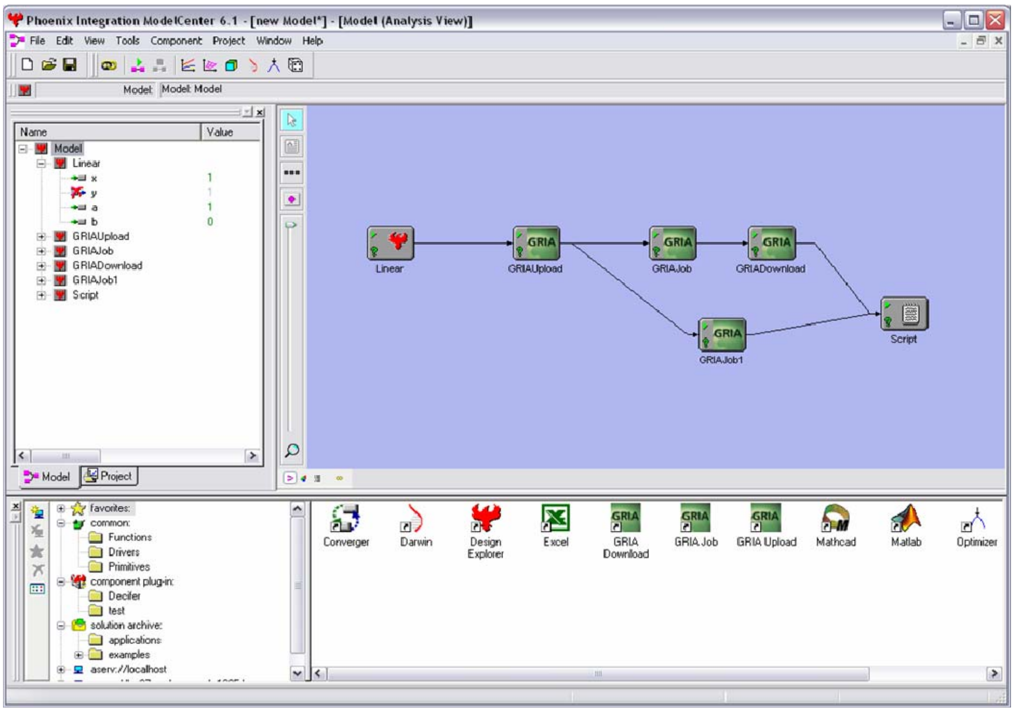


Figure 6 ModelCenter integration of GRIA services and workflows

The integration of GRIA with ModelCenter means that engineers can access distributed services and workflows from their desktop using an application they are familiar with and in a way that fits with their current working practices.

3.2.2.2 Groovy

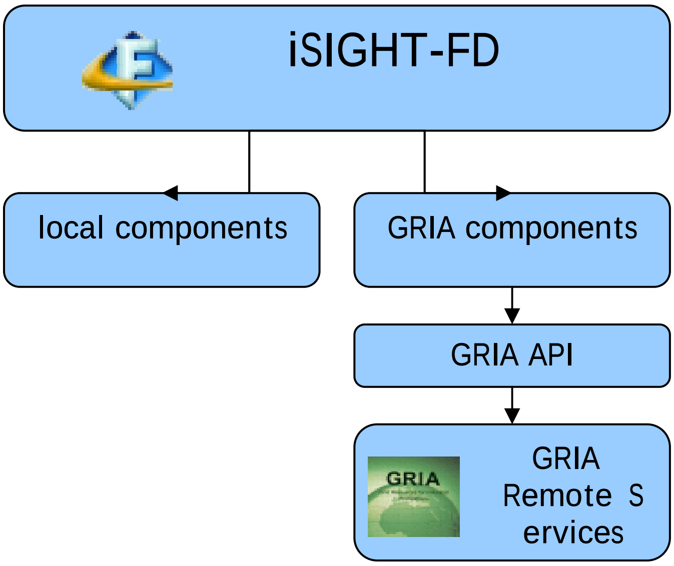
Groovy is a relatively recent dynamic language running on the JVM. The fact that GRIA is written in Java and provides a Java API makes the integration straightforward. The advantage of this integration is that it gives the opportunity to the developer to write and run his code using fast iterative loops. Hereafter is some example of GRIA usage using the GROOVY language:

```
import groovy.gria.GRIAClient

def serviceprov="https://griademo1.it-innovation.soton.ac.uk/"
def proxy =new GRIAClient(serviceprov, new File(" HTTP-proxy.properties"))
proxy.getSLAs().each{ println it }
proxy.setDefSLA("SLA for Gold Package")

proxy.getApplications().each{ println it }
def job1=proxy.createJob(" http://it-innovation.soton.ac.uk/grid/imagemagick/swirl", "my swirl")
def jobs=proxy.getJobs()
jobs.each{ println it.name}

def data1=proxy.createData("my data")
def datas=proxy.getDatas()
datas.each{ println it.name
```

3.2.2.3 iSIGHT-FD / FIPER

iSIGHT-FD is a desktop tool for engineers that provides the capability to integrate design processes, execute design studies and visualize results from those studies. When connected to the FIPER infrastructure, these model based applications can be deployed out to a user community with simple interfaces through the FIPER WebTop.

The FIPER integration with GRIA consists in developing iSIGHT-FD components to make available GRIA services in workflows, with any other components. Since components have to be written in Java, this integration is easily made with Groovy integration or Java client API.



Two different components are made available:

- a Job component : allows the engineer to run any available job, and use input and output either from files with iSIGHT-FD file manager, or from a GRIA data stager.
- a Data component : allows the engineer to move data (upload, download, copy) between URLs, GRIA data stager or Files.

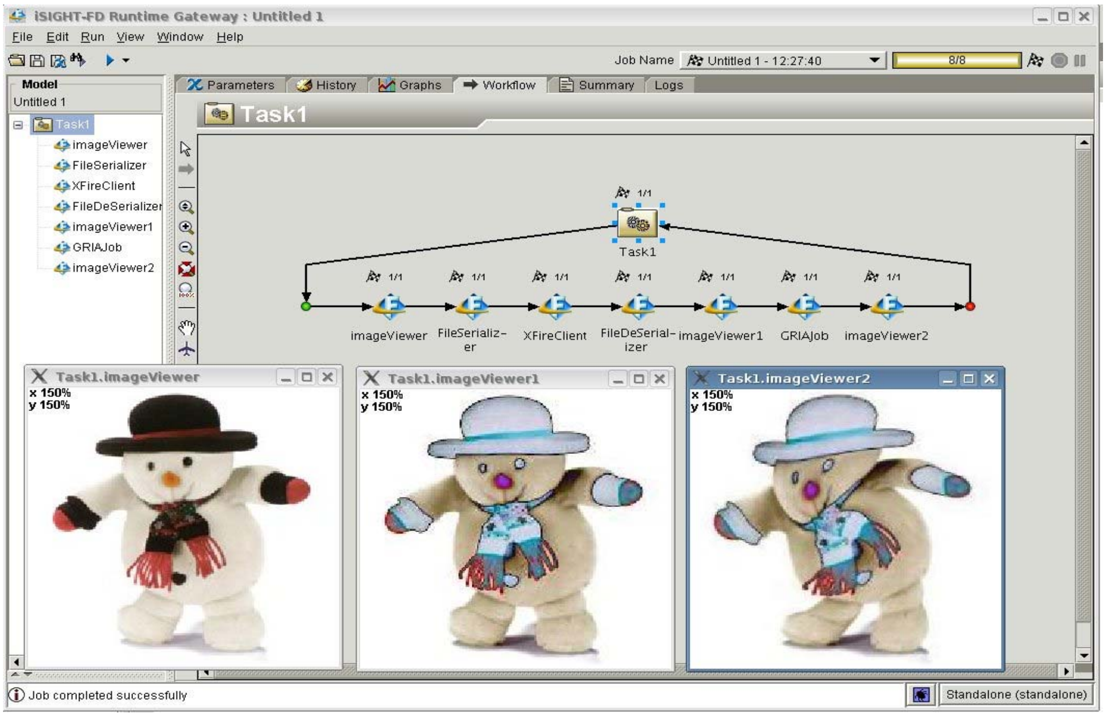


Figure 7: iSGHT using GRIA components

3.2.2.4 MATLAB

MATLAB is a popular scripting environment used by a large community including aerospace sector. Therefore MATLAB integration with GRIA services and workflows was investigated as part of the interoperability study. Improved client APIs provided by GRIA 5 releases is used in the work. With MATLAB support for Java, the system integration is relatively straightforward. Two separate Java wrapper classes were developed to represent GRIA data and GRIA jobs, respectively. Both GRIA services and GRIA workflow services are represented as GRIA jobs. These Java wrapper classes are then imported into MATLAB to access the corresponding services.

To provide the user with the same experience as other MATLAB functions, a set of MATLAB commands were developed using the Java wrapper classes. These commands are listed in Table 1.

MATLAB command name	description
gria_config	configuring the GRIA services
gria_data	construct a GRIA data object
Gria_state	create a new GRIA state repository in file or memory
gria_upload	upload a file onto GRIA service
gria_optdoe	run a design of experiment on Southampton GRIA service

Table 1 List of MATLAB commands for GRIA service and workflow access

These commands can be used in addition to the direct Java method access in MATLAB given a Java object. These tools are used in the prototype demonstrated on the second annual review. Figure xx illustrates the use of these tools from MATLAB.

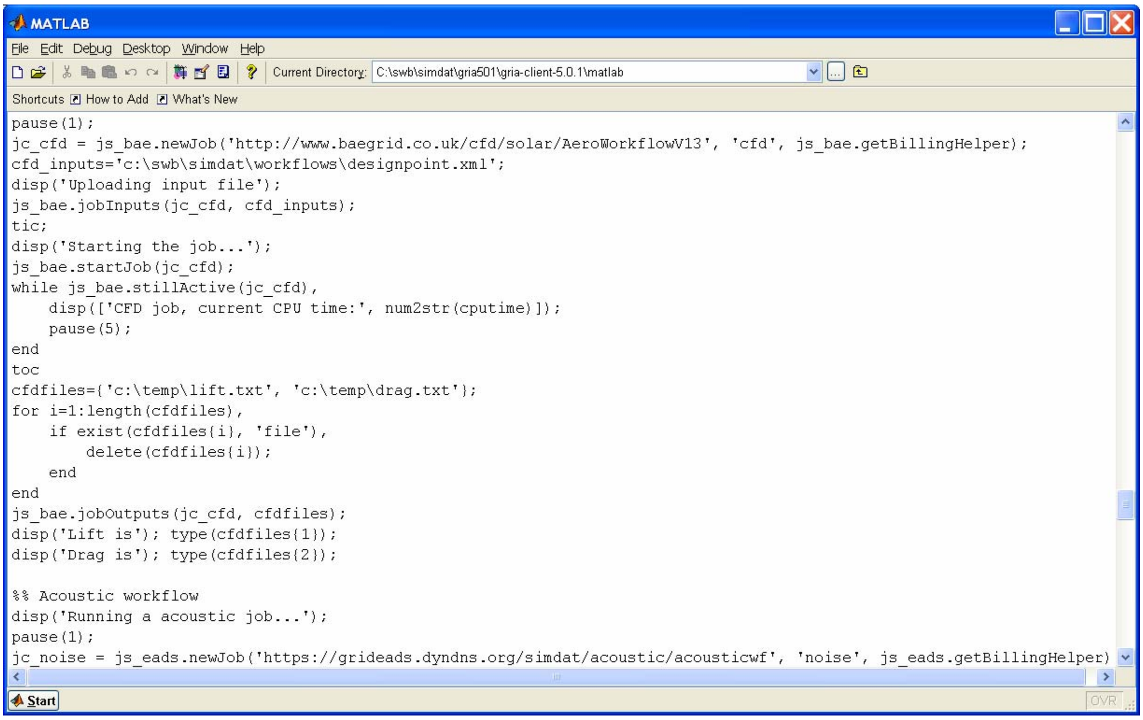


Figure 8 MATLAB integration of GRIA services and workflows

There are both advantages and drawbacks with MATLAB integration, compared with other problem solving environments with graphics user interface. The advantages include

Flexibility and ease-of-use in building complex workflows

Familiarity with engineers, and the existence of a large community

Rich functionalities in data processing and visualisation

The major drawback using MATLAB integration is the lack of 'drag and drop' workflow visual construction capability.

The approach adopted in MATLAB integration is generic and it is hoped that some of this work can be expanded to other PSEs.

3.2.3 Workflow Advisor

Since optimisation is one of the major topics in this work package, the work for workflow advisor is focused on optimisation workflows, and in particular, MATLAB workflows. The proposed framework for providing case-based reasoning capability in assistance of workflow construction is illustrated in Figure 9. The components involved are described below.

Workflow instance repository – collection of MATLAB optimisation scripts

Workflow pattern repository – collection of conceptual workflows

Component repository – collection of interested components

Case-based reasoning – reasoning engines

Aerospace CAE Design Environment – MATLAB

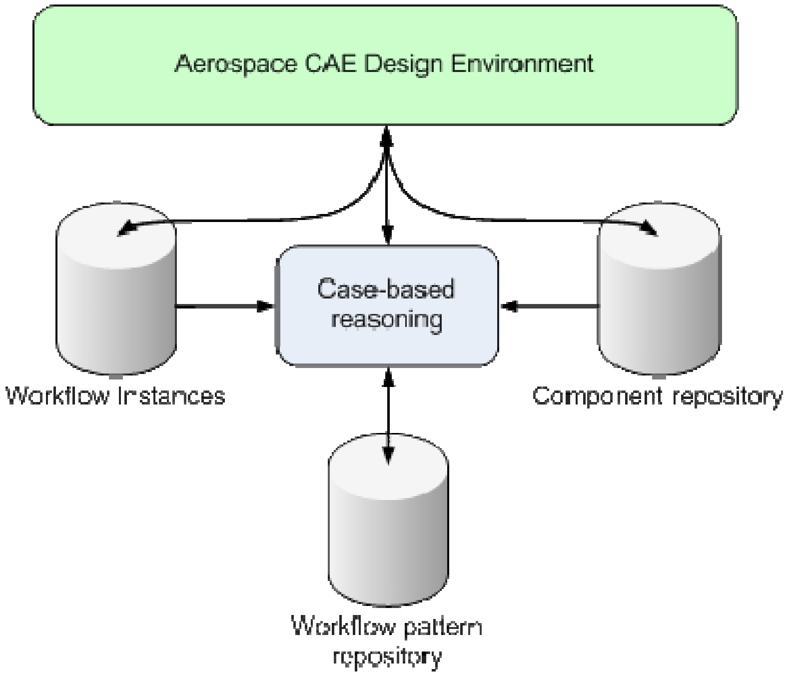


Figure 9 Proposed framework for case-based optimisation workflow construction assistant

A number of development tasks are required to implement the system. In order to extract a conceptual workflow from the workflow instances, a MATLAB parser has been developed which analyses the MATLAB scripts and extracts all the functions and variables being used in the scripts and maps them to concepts. This results in a conceptual description of the MATLAB scripts that can be compared and re-used. This work will continue into the next phase and forms part of the PM36 and PM42 deliverables.

MATLAB script parser and conceptualisation tool has become stable and is used to analyse a number of example MATLAB scripts to produce graph representations of the workflows, one such representation is shown in Figure 10.

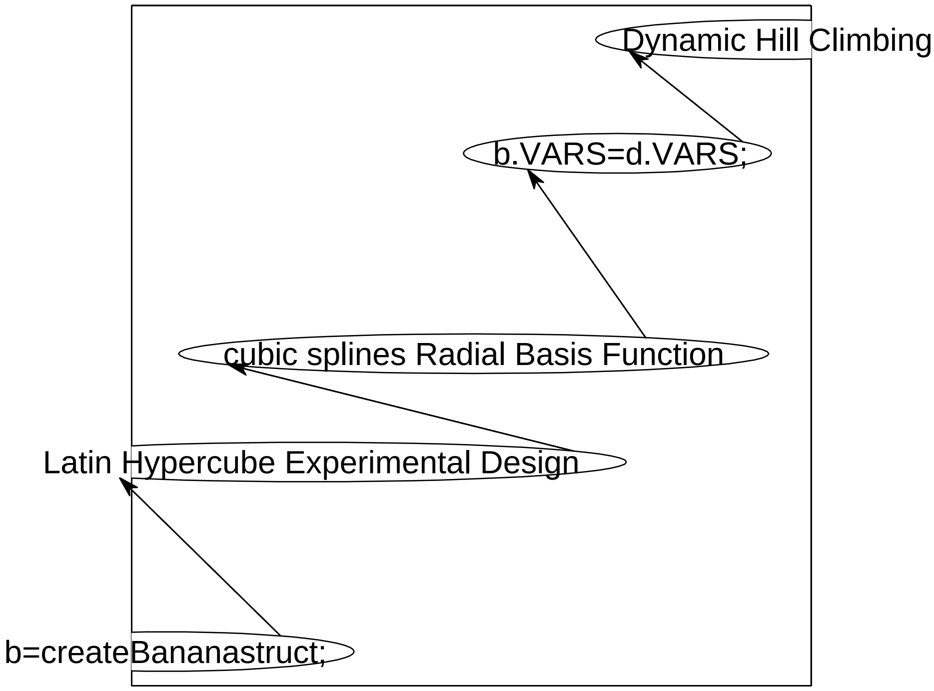


Figure 10 Graph representation of the MATLAB scripts

Further investigations are still required as to what are the best formats for these repositories and what is the best user interface for delivering this type of assistance to engineers in the aerospace industry.

3.2.4 Cost Estimation

The cost estimation scenario has been implemented using the Ontoprises Ontobroker product. To integrate all of the data sources Ontobroker runs in a distributed fashion with each instance of Ontobroker publishing its own data model based on the wrapped and annotated source data. The data models published by the distributed Ontobrokers can then be integrated and queried as a single unified data model. The instance data is then fetched from the correct source when a query is run. Figure 11 shows the architecture of the prototype.

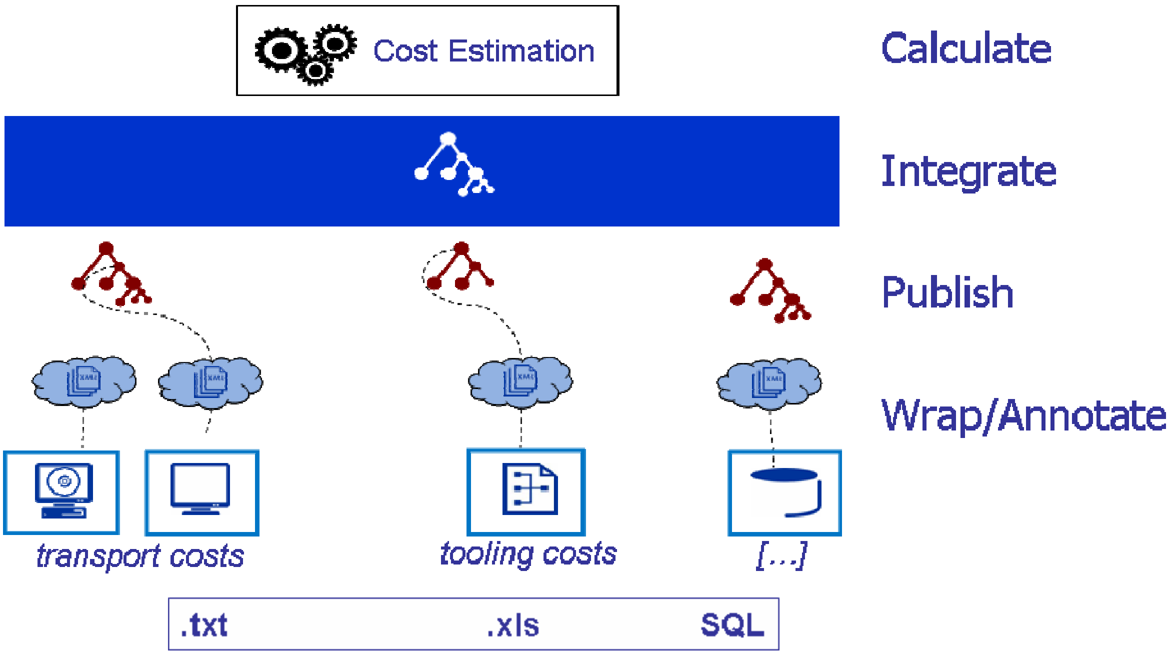


Figure 11: Cost Estimation Scenario

3.3 Deployment

The aerospace scenario is deployed using GRIA 5.01. Figure 12 shows the deployment.

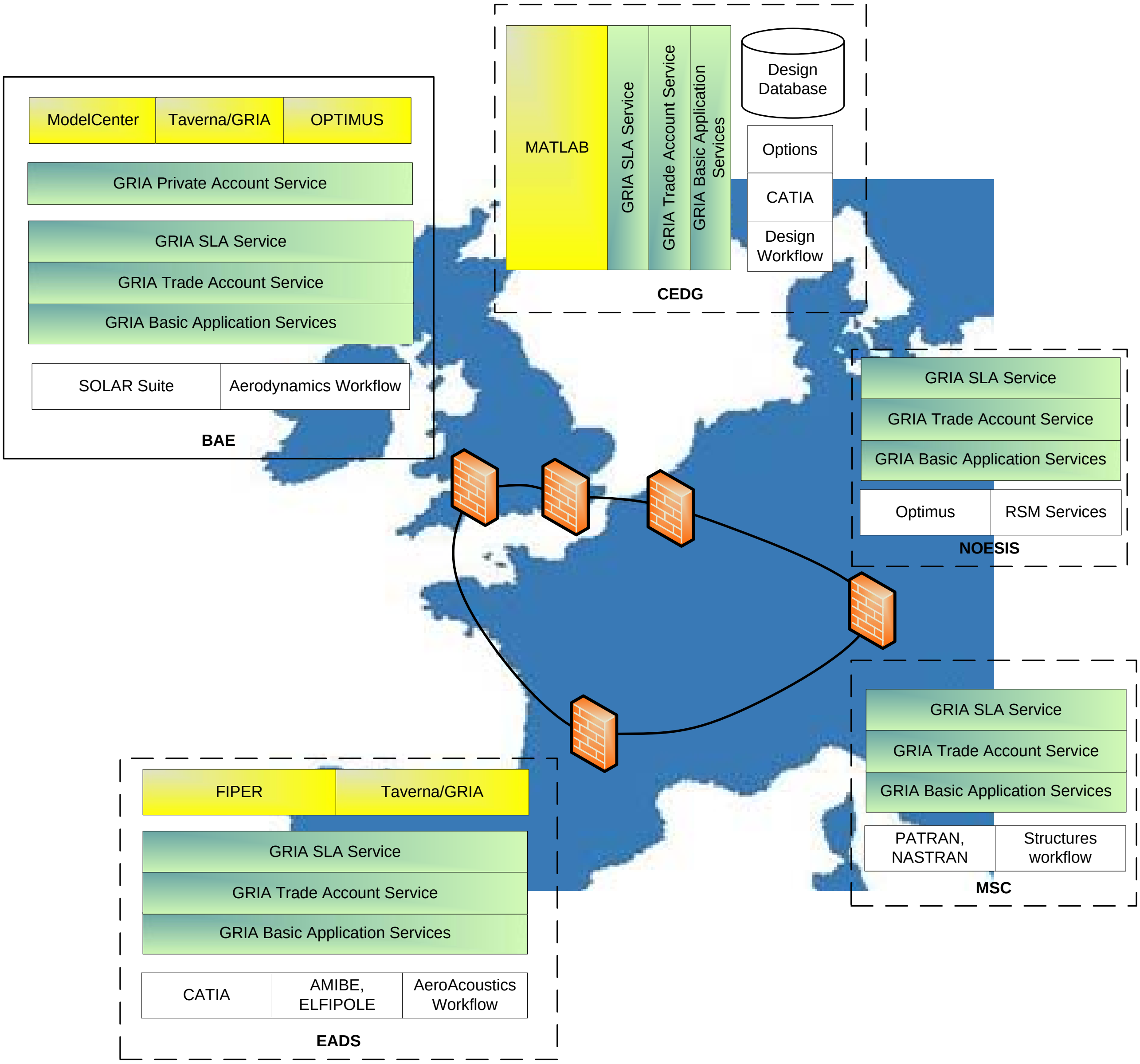


Figure 12 Aerospace Prototype Deployment

Each site has an externally accessible server with several GRIA 5.01 components installed - the GRIA5.01 basic application services, trade account service and SLA service components. The basic application services provides the job services allowing analysis jobs to be started, stopped and have their status checked as well as providing the upload and download services that allow data to be staged on and retrieved from GRIA servers. The trade account service allows users to open accounts on GRIA servers that usage can be charged to. The SLA services allow the GRIA server to propose SLA's to clients that define the service usage terms and costs. To run a job on one of the GRIA servers in the scenario a user must have an SLA in place with the service provider and an open trade account to charge that usage to. In the scenario BAE is playing the part of the prime contractor who then subcontracts the analysis services. The deployment reflects this by installing the Private Account Service at the BAE site. This allows BAE to open trade accounts and SLA's at the required analysis services and then add them to a private project account. BAE can then grant other people access to this account. So in the prototype deployment BAE manages all of the SLA's and then grants the other partners permission to run using those SLA's. As well as fulfilling the scenario this make the administration of the system simpler with only BAE required to set up accounts rather than requiring each partner to setup their own accounts and SLA's. It also allows BAE to monitor usage of all of the SLA's used within the scenario and so keep track of project costs.

BAE, CEDG and EADS all use their own PSE's to enact services. Workflow interoperability is achieved at run time by integrating the Freefluo and Optimus enactment engines with the GRIA job service. This means that workflows created in Taverna or Optimus can be published and then called from any of the other workflow environments in the scenario. For more information about the aerospace scenario workflow interoperability please see D5.2.3 [4]

3.4 Requirements status as of PM30

3.4.1 Grid Technology/Distributed Data Access

Requirement	Description	Priority	Implemented	Comment
WS-I compliant services	Standards compliant service interface	High	✓	Implemented in GRIA
Identity management services	CA, Revocation Service	High	✓	Implemented using OpenCA
Authentication service	Ability to authenticate users (X509 based) Authenticated transactions Ability to handle federated identity for exploitation phase	High	Partial	Federated identity to be looked at in next phase.
Authorisation Service	Policy driven access control to resources Dynamic policy management for exploitation phase	High	Partial	NEC's DAC technology addresses dynamic authorisation, will be looked at in a later phase.
Access to legacy applications	Service container for legacy applications including submission access to compute service	High	✓	Implemented in GRIA
Data transfer / access service	Transfer/access of flat files Database access including schema publishing in exploitation phase Policy based access control	High	✓	Implemented in GRIA
Single interface to compute service	Ability to access compute services with different scheduling requirements through single interface Reservation of compute resources Sandboxing runtime in compute service including ability to specify sandbox environment	Medium	Partial	Reservation and sandboxing
Resource discovery	Ability to discover alternate services due to service failure or	Low	Partial	Failover functionality

	unavailability			available in Taverna and Registry planned for next GRIA release

3.4.2 Administration of Virtual Organisation

Some of the requirements for the administration of the Aerospace Activity virtual organisation are also covered by in the Grid Infrastructure requirements section

Requirement	Description	Priority	Implemented	Comment
Identity management services	Ability to create and manage user digital identities	High	✓	Implemented using OpenCA
Authentication service	Ability to authenticate users Authenticated transactions Ability to communicate securely Ability to handle federated identity for exploitation phase	High	Partial	Federated identity to be looked at in next phase.
Authorisation Service	Policy driven access control to resources Dynamic policy management for exploitation phase	High	Partial	NEC's DAC technology addresses dynamic authorisation, will be looked at in a later phase.
Resource discovery	Ability to discover alternate services due to service failure or unavailability	Low	Partial	Failover functionality available in Taverna and Registry planned for next GRIA release
Auditing	Execution and resource audit for QA purposes	High	Partial	Provided but not validated against Organisational policy
Accounting	Ability to charge for service	Medium/Low	Partial	Not linked to

	provisioning			payment systems

3.4.3 Workflow

Requirement	Description	Priority	Implemented	Comment
Workflow access to web services and resources	Workflow composition tool needs to have the ability to dynamically access web services including links to Authentication and Authorisation services	High	✓	Provided by Taverna-Freefluo/GRIA
Ability to handle long duration process	Services can have long duration (order of 1 week). Ability to check progress by polling/notification therefore required. Ability to close workflow tool and return to check state also required.	High	✓	Provided by Taverna-Freefluo/GRIA
Exception handling	Ability to specify behaviour due to service failure, connectivity failure, decision points, user intervention	High	✓	Provided by Taverna-Freefluo/GRIA
Remote batch execution of workflow	Ability to submit workflow to be remotely executed Workflow enactor as a service	Medium	✓	Provided by Taverna-Freefluo/GRIA and Optimus
Parallel workflow execution	Ability to execute the workflow in parallel (same workflow executed with a range of inputs simultaneously)	High	✓	Available in Taverna and Optimus.
Workflow execution optimisation	Control of workflow execution with constraints of service availability	Medium/Low	×	

Workflow publishing	Ability to publish workflow via a web portal	Medium	✓	
Workflow mining	Ability to search workflow database using meta-data	Low	×	
Workflow language interoperability	Ability to exploit workflows in other standards based workflow enactors	Medium	Partial	Only when workflows are accessed as GRIA services. Runtime interoperability
Abstract workflow construction	Ability to construct workflows using abstract service descriptions	Medium	×	
Abstract workflow execution	Ability to execute abstract workflows with runtime binding to services via a semantic service registry	Medium	×	
Workflow composition advisor	Ability for the workflow authoring tool to advise users on next steps based on prior knowledge in workflow repository	Medium	×	

3.4.4 Analysis Services

Requirement	Description	Priority	Implemented	Comment
Analysis service control	Ability to control service (run, suspend, stop) using web service interface	High	✓	Provided by GRIA
Access to intermediary output	Ability to monitor process output during execution (stout, stderr, files) depending on access control policies	High	✓	Provided by GRIA
Polling and or notification	Ability for client to poll state or for client to register a callback mechanism (SMS, email, callback service)	High	✓	Provided by Taverna

Auditing	Execution and resource audit for QA purposes	High	Partial	Log data provided but this has not been verified against organisational policies
QoS measures	Ability to describe quality of service provided by analysis service	Medium /Low	✓	GRIA SLA mechanism.
Accounting	Ability to charge for service provisioning	Medium /Low	Partial	Provided by GRIA but not linked to payment system
Access to results	Policy controlled access to results	Medium	✓	Provided by GRIA
Results lifetime	Ability to specify lifetime of results	Medium	Partial	Limited capability provided by GRIA
Semantic description of analysis service	Ability to semantically describe analysis service (inputs/outputs/behaviour) to facilitate deployment and to enable the exploitation of semantic service registries	High	×	Registry planned for next GRIA release

3.4.5 Ontologies

Requirement	Description	Priority	Implemented	Comment
Ontology construction	Ability to create appropriate and extendable ontology for scenario test case describing the product as well as the concepts in the design process	High	✓	Provided by Ontobroker, demonstrated in cost modelling scenario.
Ontology interrogation	Ability to interrogate the ontology to extract information	High	✓	Provided by Ontobroker.
Ontology driven data access	Ability of knowledge service to access ontologically described	High	×	

	data			
Multiple data source access	Ability of semantic mediator to access data held in a variety of data formats/sources.	High	✓	Provided by Ontobroker, demonstrated in cost modelling scenario.

3.4.6 Knowledge Services

The work on knowledge services is based on the cost modelling scenario and builds on the work done in the ontology's work package to allow the knowledge services to be run through a semantic layer to integrate a variety of data sources. This is ongoing work and will be more fully addressed in the next phase.

Requirement	Description	Priority	Implemented	Comment
Cost Prediction	Ability to estimate future costs based on historic cost data.	High	×	
Knowledge services	Ability to access knowledge tools as services.	High	✓	WEKA toolkit available as GRIA services
Distributed knowledge access	Ability to access data held in OGSA-DAI databases	High	✓	WEKA toolkit can access data held in OGSA-DAI.
Multiple source data integration	Ability to search across a variety of data sources i.e. OGSA-DAI, flat file, excel spreadsheets.	Medium	×	
Distributed knowledge aggregation	Ability for a member of the VO to access aggregated knowledge about the whole problem using ontology described data to generate aggregated knowledge that is not otherwise visible to a single team, organisation or specialism	Medium/Low	×	

3.5 Validation

The validation of this phase of prototype was carried out by the end users at each of the organisations in the VO. The aim of this phase was to extend the connectivity phase scenario to demonstrate interoperability. To validate the prototype we will look at the functionality provided and success of the deployment as well as validating against the list of stated requirements.

In section 5.4 the requirements of the PM30 prototype are listed along with their current status. The table below shows a summary of the number of requirements met, partially met or not met.

	Yes	Partial	No
Grid Infrastructure	4	4	
Virtual Organisations	1	5	
Workflow	6	1	5
Analysis Services	5	3	1
Ontologies	3		1
Knowledge Services	2		3
Total	21	13	10
	47%	30%	23%

From this table you can see that the majority (77%) of the requirements were met or partially met. For those only partially met a shortfall has been identified and in the majority of cases a way forwards proposed. 23% of the requirements were not met, there requirements are discussed in section 5.6. Only 2 High priority requirements were not met – the Semantic registry which is planned for the next GRIA release and the cost prediction using knowledge services which is discussed in SIMDAT deliverable D8.2.3 [5].

The functional validation of the prototype in summed up in the table below. The table shows the partners involved in the prototype and their status against a set of functionalities.

	BAE	EADS	UoS	MSC	NoESIS
Hosting GRIA 5.01 Services	Yes	Yes	Yes	Yes	Yes
GRIA Services external accessible	Yes	Yes	No*	Yes	Yes
GRIA Client	Yes	Yes	Yes	Yes	Yes

access to aerospace services.					
Analysis Service SLA in place.	Yes	Yes	Yes	Yes	Yes
Analysis service workflows deployed	Yes	Yes	Yes	Yes	N/A**
PSE Integration	ModelCenter	FIPER	MATLAB	N/A***	Optimus

(*) Due to firewall restrictions and CATIA licensing some services can only be called from UoS but the optimisation is being driven from UoS and so the scenario is unaffected.

(**) NoESIS were just providing individual RSM services and not a full analysis service workflow.

(***) MSC were acting the part of a service provider in the scenario and so no problem solving environment was integrated.

3.6 Outstanding Issues

Outstanding issues from the PM30 prototype are the service registry and the integration of the semantic integration work with the knowledge services.

The service registry was explored and several options were investigated. A service registry is planned for the next release of the GRIA software and the aerospace prototype will be upgraded to use this new version.

The integration of the knowledge services in the cost modelling scenario was delayed due to staffing issues but an architecture was defined and a way forward proposed. For more information see SIMDAT deliverable D8.2.3 [5]

3.7 Summary

The objective of this phase of the project was to demonstrate interoperability within the system. In order to demonstrate this the connectivity phase use case was extended, the use case required analyses from experts across disparate design teams and organisations.. We chose to simulate the multi-disciplinary collaborative configuration design of a low-noise, high-lift landing system. The scenario is typical of sub-system design problems in the context of, say, future-concept, unmanned cargo vehicles that require an ability to use airfields in noise-sensitive locations. It requires issues such as design, aerodynamic performance, acoustic performance and structural performance to be considered. The prototype was deployed using the latest version of the GRIA toolkit that allowed individual groups working on their own services to link their software to other groups in different companies in order to form virtual organisations that were both secure and accountable. The new

SLA model and private account service allowed the VO to adopt the business collaborative collaboration pattern that closely matched the described scenario.

The integration with the commercial problem solving environments proved very successful and each partner in the aerospace activity was able to integrate with the PSE used within their organisation. This demonstration of integration is extremely useful as it shows how the SIMDAT grid technologies can be used in existing environments. Showing this enables engineers in the organisation to quickly see how they could use Grid technology within their existing design processes.

The prototype has successfully demonstrated interoperability and we now want to move on to looking at the challenges presented by making better use of the knowledge embedded in the analysis services and prototype workflows. The cost modelling scenario and a prototype produced that successfully demonstrated the use of semantic technologies in integrating a variety of data sources.

4 Description of the next prototypes (PM36 and PM42)

The next phase of the project is the knowledge phase. For this phase we will be looking at how we can make better use of the knowledge generated in the system. There will be no change to the PM24 use case and scenarios. Within the prototype we are dealing with two types of knowledge – process and product knowledge. Product knowledge is the knowledge at the analysis service level and process knowledge is the knowledge behind the construction of the workflows. In the aerospace activity this is focused on optimisation workflows.

The aim of making use of the knowledge is to try and reduce the total time of the simulation and demonstrate knowledge reuse with an optimisation workflow construction advisor system. We will look at expanded use of RSM'S, high/low fidelity simulation and intelligent data management. We will also be implementing system verification and testing system to test the availability and performance of the system.

4.1 Product Knowledge

Each analysis service workflow is currently constructed by the expert in that particular discipline; it is that expertise that we want to imbed in the workflows to make intelligent decisions within the workflows. As an example of this please see figure 13.

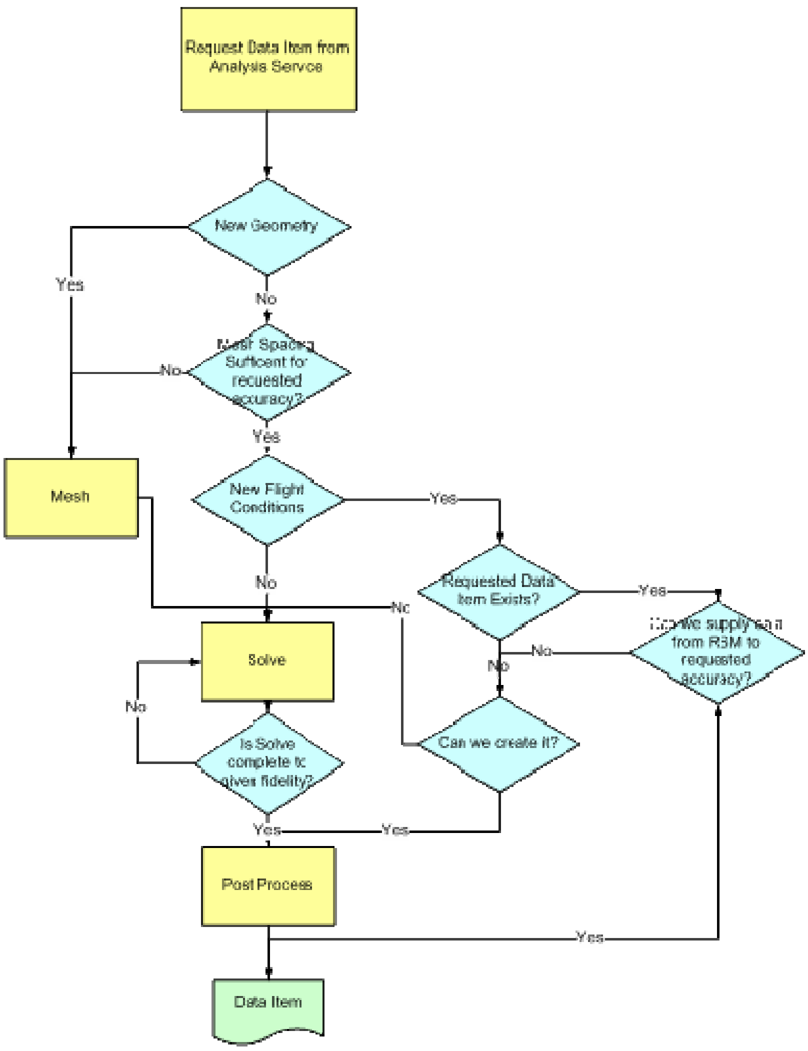


Figure 13 Product Knowledge Workflow example

In this workflow the requested data item is examined and comparisons to existing data items made to see if they can be reused or approximations can be made using existing data. For this kind of workflow to be possible we need a good understanding of the data in the system. This means the first step to creating these enhanced workflows is an analysis of the existing workflows to identify the data flows, data provenance and life times. This analysis will enable us to answer questions along the lines of “the requested data item does not exist, can we create it from existing data items?” Another important addition to this workflow is the ability to extract data from the output of a job to monitor how the analysis is progressing. In the above example this involves monitoring the residuals and making decisions on the convergence of the solver. Using this you could then decide whether to carry on with the solver or to stop it.

To be able to use the data of previous analysis we need some way of managing the data in the system. This data management layer will need to be able to reference files in a file system and also hold metadata about those files. This data will be held at each analysis service but access to this data may be required from another site, for example the noise sources are shared between the aerodynamics and acoustic services, so the data will have to be accessible in a distributed fashion.

4.2 Process Knowledge

The process knowledge work will focus on the creation of a workflow advisor. The workflow advisor aims to provide assistance to end users when new workflows are being built. The focus of the work is on design workflows – workflows that use various optimisation methods and strategies to improve designs. MATLAB script has been identified as suitable design optimisation workflows for prototype and will be used to demonstrate the use of various knowledge technologies.

The framework for the prototype is described in section 3.2.3, in which, the workflow instances and workflow components are stored in repositories. The MATLAB parser and conceptualisation tools are used to analyse the MATLAB scripts and extract component usage patterns in the workflow. The workflow patterns will then be archived in a repository of conceptual workflows. These repositories, combined with a reasoning engine, will form the basic components for optimisation knowledge modelling framework.

The prototype will be based on a continuation of work from PM30 and enhanced with revised optimisation ontology. It is expected that the combination of workflow analysis and ontology will allow different workflow instances to be compared on conceptual level and to provide answers to the following example questions:

- Is there any similarity between the two workflow instances?
- Is a particular component used by a workflow instance?
- What is the most likely component being used after a particular component?
- Locate the workflow instances that use one component?

Repositories of workflow instances and conceptual workflows will be established and populated with representative workflows. Combined with reasoning capabilities provided by ontology, the prototype will be used to demonstrate that knowledge technology can provide required support for making informed decisions when constructing design workflows for aerospace applications. The tool will be deployed in the MATLAB environment.

4.3 Validation and system metrics

In the next phase, we will also define metrics in order to characterise the Aerospace grid. A validation process will be used in order to automatically evaluate the connectivity and performance of the Grid. For this task, a set of services will be deployed on the sites of the Aerospace grids; these services will be used in order to assess the Quality of Services (QoS) of the various sites. This will provide a kind of Weather Service for the aerospace grid. As the GRIA middleware comes with a tutorial based on various imaging jobs, the Weather service will probably rely on such jobs. Among the foreseen metrics are:

- Maximum roundtrip time for a job,
- Execution time for a job,
- Maximum roundtrip time for a given workflow.

Simultaneously some work will be devoted:

- To check how job instances conform to the SLAs proposed by the sites. This information could be used to rank the different sites proposing similar services,
- To assess the use of a Grid based optimisation process as compared to the former processes that were used in the aerospace industry.

5 Resulting requirements

Name	**Metadata for services and workflows**		
Req. Id	AERO-001		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	Southampton CEDG	Technology component	Workflow
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Adding metadata for published services and workflows • ontology support for metadata • API access to the metadata from workflow authoring environments			
Validation			
• Ability of users of workflow composition tools to add ontology enhanced metadata to services and workflows			
Assumptions			
•			

Name	**Ontology Support for Workflow Composition**		
Req. Id	AERO-002		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High

Created By	Southampton CEDG	Technology component	Workflow, Ontology
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Definition of workflow ontology • API access to the ontology from workflow authoring environments			
Validation			
• Availability of ontology to workflow authoring environments			
Assumptions			
•			

Name	**Workflow Repository**		
Req. Id	AERO-003		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	Southampton CEDG	Technology component	Workflow, Grid Infrastucture
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Relation to prototype			

• Aero PM42			
Requested functionality			
• Workflow repository conforming to standards • Archival of workflows into repository from workflow authoring environments • Retrieval of workflows from repository from workflow authoring environments • API accesses to above functionalities			
Validation			
• Ability of users of workflow composition tools to query, search workflow repository, in addition to the ability to add new workflows into repository from workflow authoring environments			
Assumptions			
•			

Name	**Product Knowledge Workflow Components**		
Req. Id	AERO-004		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES	Technology component	Grid Infrastructure, Workflow.
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Ability to add local components into workflows to make decisions based on product knowledge.			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Each partner able to author they're own custom workflow decision nodes. • These nodes must be deployable in published workflows.			

Validation			
• Ability of users to create nodes and demonstrate path through workflows being affected by product knowledge decisions.			
Assumptions			
•			

Name	**Product Knowledge Workflow Monitoring Components**		
Req. Id	AERO-005		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES	Technology component	Grid Infrastructure, Workflow.
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Ability to add local components into workflows to make decisions based on the output of currently running jobs and have the ability to stop that job based on product knowledge.			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Each partner able to author they're own custom workflow decision nodes. • These nodes must be deployable in published workflows. • A node that is able to monitor the output of a GRIA job and change the state of that job before it finishes/fails.			
Validation			
• Ability of users to create nodes and demonstrate a GRIA job being stopped or restarted with different inputs based on a decision made in a node monitoring it's output.			
Assumptions			
•			

Name	**Data Lifetime Management**		
Req. Id	AERO-005		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES	Technology component	Grid Infrastructure, DDRA.
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Ability to associate data life times to data items.			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Each item of data within the system to have an associated lifetime, once this lifetime is reached the data is automatically removed.			
Validation			
• Removal of data beyond it's lifetime.			
Assumptions			

Name	**Data Management**		
Req. Id	AERO-006		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES	Technology	Grid Infrastructure,

		component	DDRA.
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Ability to store file references and associated metadata in a data management system.			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Each analysis service is able to store required data items and related metadata and query that metadata to retrieve the data items at a later date.			
Validation			
• Storage and retrieval of data at the analysis service level.			
Assumptions			

Name	**Distributed file access**		
Req. Id	AERO-007		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES	Technology component	DDRA
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Ability to share files between analysis services.			
Relation to prototype			

• Aero PM42			
Requested functionality			
• Ability to use IGORFS with GRIA to share analysis data between analysis service nodes.			
Validation			
• Access of Lighthill sources from BAE by EADS over IGORFS			
Assumptions			

Name	**Surrogate Data Models**		
Req. Id	AERO-008		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES	Technology component	Knowledge
Status	New requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Extended use of surrogate data models in analysis services.			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Each analysis service to be able to use RSM's to give analysis solutions based on previous data.			
Validation			
• Demonstrated extended use of RSMs in scenario			

Assumptions			
•			

Name	**Authentication Service**		
Req. Id	AERO-009		
Application Activity	Aerospace		
Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	Medium
Created By	BAES, EADS	Technology component	Grid Infrastructure, VO
Status	Existing Requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Ability to integrate GRIA authentication services with existing enterprise schemes.			
Relation to prototype			
• Aero PM42			
Requested functionality			
• Ability to authenticate to GRIA using enterprise identity scheme.			
Validation			
• Ability to authenticate to GRIA using enterprise identity scheme (i.e. LDAP or MS Active Directory)			
Assumptions			
•			

Name	**Semantic Registry**
Req. Id	AERO-010
Application Activity	Aerospace

Prototype(s)	Aerospace prototype for PM42		
Date Created	2007-03-27	Priority	High
Created By	BAES, EADS	Technology component	Grid Infrastructure
Status	Existing Requirement		
First Implementation Date	End of August 2007	SIMDAT module targeted	WP 11.3
Description			
Semantic Registry for Job Services			
Relation to prototype			
• Aero PM42			
Requested functionality			
Need for semantic registry to locate and describe deployed job services.			
Validation			
• A deployed registry in the aerospace scenario			
Assumptions			

6 Conclusion

The PM30 prototypes successfully fulfilled the aims of the interoperability phase of the project. The phase one scenario was successfully extended to include new services and introduced new partners to the VO. The adoption of GRIA 5.01 allowed the use of the new SLA based service agreements and allowed the adoption of the business cooperative VO model that more closely matches the aerospace business requirements. The prototypes successfully demonstrated the integration of several commercial PSE's with the Simdat technologies, showing how these technologies can be used within existing engineering processes. The prototypes also successfully demonstrated runtime workflow interoperability, showing how experts in the individual domains can author workflows in their tools but enable access to those workflows through a neutral GRIA interface. The cost estimation scenario successfully demonstrated the use of semantic technology in providing access to distributed and heterogeneous data. The semantic layer shows how new supplier data could quickly be integrated and considered when performing a cost estimation.

As the project moves into the knowledge phase the aerospace activity will be looking at making better use of the knowledge within the system. By examining the data flows within each analysis service and looking at the extended use of surrogate data models we hope to decrease the total analysis time of the system. We will also be looking at the process knowledge in the system to produce a workflow advisor system that can make better use of the process knowledge in the system to advise users when constructing optimization workflows. Also in the next phase constant system validation will be undertaken to monitor performance of the system and the availability of the services.

7 References

1 SIMDAT Annex I - “Description of Work”
2 Prototype System Description and Capability D11.2.2
3 Initial version of the application scenario, demonstrating connectivity and the operation of the model problem, SIMDAT deliverable D11.2.1
4 Consolidated Report on Implementation of Workflow Management Infrastructure, on Workflow Interoperability and Business Processes and on Meta-scheduling design, SIMDAT deliverable D5.2.3
5 Report on design of data mining tools for Workflow and Aerospace. D.8.2.3

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