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

D.15.4.8 Corus Demonstrator Evaluation

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RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	X

Revision history

Date	Version	Author	Modification
1/10/2008	0.1	Mike Boniface	Initial outline version
16/10/2008	0.2	Ken Meacham (IT Innov) Didier Farrugia (Corus)	Overall description of scenario, technologies and deployment
3/11/2008	0.3	Boon Cheong (Corus)	Updates to Chapter 8, plus new screenshots
5/11/2008	0.4	Didier Farrugia (Corus)	Updated benefits and conclusions
10/11/2008	1.0	Mike Boniface	Final QA and review

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1 Overview

This document is the deliverable D.15.4: Corus Demonstrator of the EU IST-2002-511438 SIMDAT project, as specified in the Annex 1 - "Description of Work".

The SIMDAT Grid Solution Portfolio has been developed to meet the needs of industrial partners undertaking the collaborative design of complex products in four application sections; aerospace, automotive, meteorology and pharmaceutical. The portfolio consists of Grid technologies supporting both infrastructure (security, management, discovery, data access, execution and workflow) and application (problem solving environments and analysis tools) capabilities.

The purpose of this demonstrator project was to deploy appropriate parts of the SIMDAT Grid Solution Portfolio within an application sector not currently exposed within the SIMDAT project, in order to validate the portfolio as a framework for building domain-specific Grid solutions. Corus RD&T therefore joined the EU IST SIMDAT project as a subcontractor in order to evaluate the application of the portfolio to the design and analysis of complex products and thermal-mechanical processes in the steel industry.

This document describes the Corus Demonstrator scenario, and how this fits into the Corus business context. The motivation for using SIMDAT tools is also highlighted, together with the selected SIMDAT technologies employed, their setup and integration. Finally, the project results are evaluated, in terms of any challenges that were raised or overcome, along with an analysis of the benefits of using the SIMDAT Grid Solution Portfolio over current methods.

2 Demonstrator Description

2.1 Introduction

This section introduces the end-user partner, Corus, describing their application sector and motivation behind their involvement in the demonstrator. We then go on to describe the Corus scenario and use cases in more detail.

2.2 CORUS

Corus is an international company, providing steel products and services to customers worldwide. Corus is Europe's second largest steel producer with annual revenue of around 12 Billion pounds and a crude steel production of over 20 million tonnes. Corus is part of the Tata Steel Group. Corus supplies innovative solutions and products to a broad range of markets such as aerospace, construction, energy and power generation sector, engineering, packaging and rail. The Research, Development and Technology (RD&T) business of Corus combines top class innovation with cutting edge technology to deliver 'metals solutions' in a constantly changing world. Corus continually upgrades manufacturing processes and uses the latest methods in process analysis and design, product design, modelling/simulation, and prototyping and application development. Large-scale test facilities permit new products to be tested on an industrial scale, such as can making, production of blanks for car parts, brazing of aluminium radiator elements and corrosion testing of civil constructions.

Corus employs almost 950 researchers across Britain and the Netherlands and supply 'metal solutions' to Corus sites around the world. Corus works in collaboration with universities and research institutes all over the world as well as with key customers in the automotive, transport, packaging and construction areas.

2.3 Motivation

The steel manufacturing process is complex and lengthy, involving at least 10 primary sequential processes from ironmaking, steelmaking to coating. Each process can be broken down into sub-processes that have both product and process parameters that affect the evolution of microstructure, as well as the final properties. Key parameters, from shape to microstructural properties such as grain size, have to be taken into account and transferred from one process to the next and their effect analysed within the constraints of the process. This field is known as through-process modelling (TPM). The ultimate goal is to be able to understand which manufacturing process drives which properties (i.e. sensitivities) but also to predict the final microstructure and associated properties for current and future steel grades. TPM is also used for harnessing the value of combining representative models in order to further improve their accuracy as well as easing integration and use of legacy and newly developed internal or external simulation models. Combining heterogeneous techniques (analytical, discrete) and physical length scale, together with distributed computing, is also a key driver for embracing TPM and workbench technology. For this reason, Corus are always keen to embrace any new technologies that might help to give them the competitive edge over rivals in the steel industry.

Corus has many years of experience in the TPM field, and have worked closely with IT Innovation in the past, through projects within the ECSC framework, to develop “workbench” technology to integrate various in-house simulation and analysis tools. Since this initial collaboration, technology has progressed, including the development of new problem solving environments (PSEs) and workflow tools, plus the means to orchestrate the execution of processes either locally, on remote resources within the company, or even to outsource to remote suppliers of application services.

Corus are keen to make best use of computational resources within their organisation, and see GRIA as an attractive tool for enabling this. GRIA provides a generic environment to enable access to remote applications either within their company (utilising spare computational resources and intranet deployment), to partner sites around the world (e.g. TATA, their parent company), or to outsource to external application suppliers.

They have experience of using iSight-FD® with customised, internally developed, agents/services for remote execution, of jobs on LINUX clusters. However, the cost of licensing for full FIPER services support within RD&T (and possibly Business Units) is a concern for deploying TPM technology more effectively within the Company. GRIA has the potential to provide remote job execution for Corus engineers, but also has the advantages of providing security of data plus business-to-business (B2B) functionality that enables collaborations to be set up easily. Of course, as GRIA is also free to download, and commercial support is available, this adds significantly to its attractiveness to Corus.

Corus were therefore keen to evaluate SIMDAT technologies, in particular to see how GRIA job execution could be built into their current workflow tool, iSight-FD®, via GRIA plugins developed by EADS.

2.4 Corus Demonstrator Scenario (Test Case)

The Corus Demonstrator scenario consists of a through process modelling (TPM) workflow, to simulate transient cooling, followed by a solid state transformation to room microstructure. An initial cooling step simulates natural air cooling of a 180x180x51kg/m I-beam section in the I position (Figure 1 single step cooling of 1500s from an initial temperature of 800°C). This is followed by sequential modelling of the solid state phase transformation for one specific point of the I beam section.

The initial cooling step produces an output mesh, which is post-processed to produce a [Time, Temperature] array at one single specific node of the mesh. This temperature array is used as input to the solid state model.

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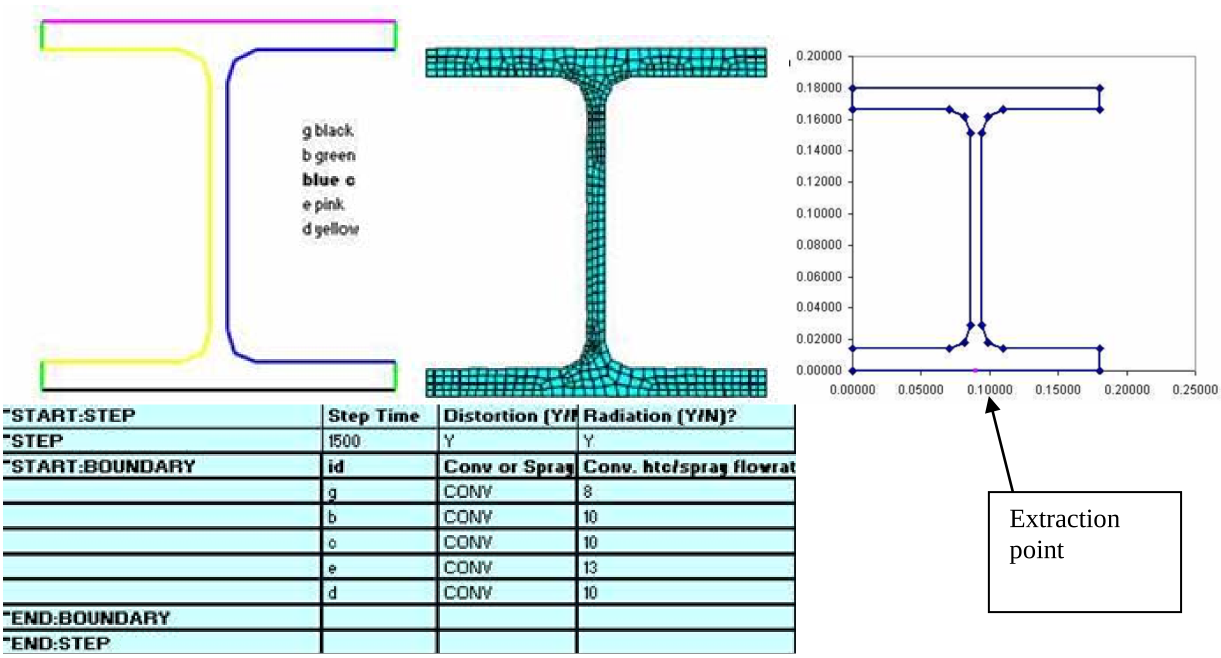

*START:STEP	Step Time	Distortion (Y/I	Radiation (Y/N)?
*STEP	1500	Y	Y
*START:BOUNDARY	id	Conv or Spray	Conv. htc/spray flowrat
	g	CONV	8
	b	CONV	10
	c	CONV	10
	e	CONV	13
	d	CONV	10
*END:BOUNDARY			
*END:STEP			

Figure 1: FEHT set-up 180x180x51kg/m natural air convective cooling

Temperature contours of FEHT simulation without transformation are shown in Figure 2. (From an initial temperature of 800°C.) Typical CPU time for 1500s cooling is approx 3s. Figure 3 shows a cooling curve at a node of interest with/without effect of coupled transformation. It should be noted that rigorous analysis of transient cooling from austenite to room temperature should be carried out in a fully coupled mode.

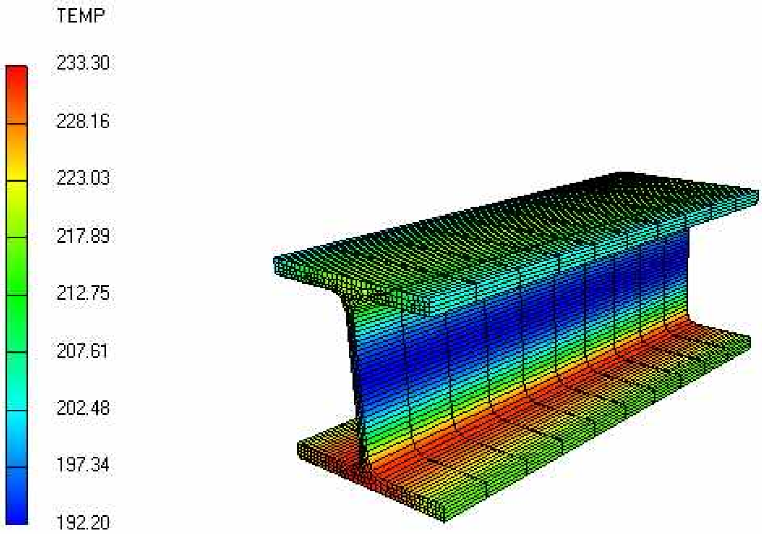

Figure 2: Temperature contour predicted by FEHT (decoupled to phase transformation)

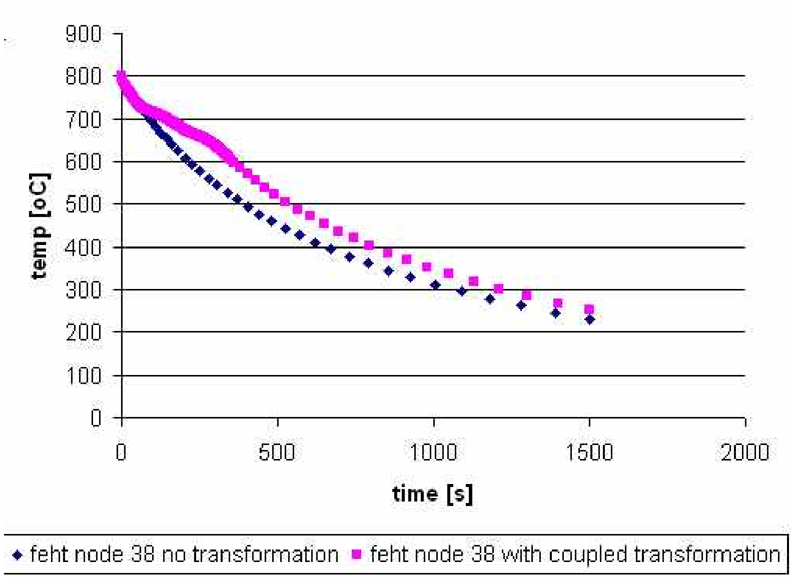

Figure 3: Temperature-time with/without fully coupled transformation at node of interest

2.4.1 CamModel

CamModel is a solid state phase transformation model used in previous Steel Modelling Workbench ECSC project.

In the context of this proposal, CamModel has been used with the following input CamInput.dat file, allowing reading of time, temperature data from a .txt file (see input below), therefore modelling uncoupled transformation (i.e. transformation not affecting temperature via latent heat of transformation).

"testgria1.out"

.17,0,1.4,0,0,0,0,0,0,0,0,0,0

20,0,0

6

"templ.txt"

0

2.5 Corus Demonstrator Set-up Phases

For the two main stages in this TPM scenario, Corus have previously used their proprietary 2D FEM Fortran 90 thermal heat transfer code (FEHT), and their solid state physical phase transformation model, CamModel, respectively. However, the aim of this project was to demonstrate the outsourcing of the cooling simulation step of the TPM scenario to an external application provider, via SIMDAT technologies coupled to their favoured workflow tool, iSight-FD®.

As this set-up was relatively complex, it was broken down into a number of phases, as described in the following sections.

2.5.1 Phase I – Local FEHT execution

Phase I of the demonstrator set-up consisted of wrapping the Corus (in-house) applications (FEHT and CamModel) as iSight-FD® components, such that they could be built into an iSight-FD® workflow. For this, Corus used version 2.5-2 of iSight-FD®.

Both models were wrapped within the iSight-FD® environment and an iSight-FD® data exchange manager component was also constructed, to provide a suitable template and file extension (.txt) as the input to the CamModel execution step. The resulting iSight-FD® workflow is shown in Figure 4

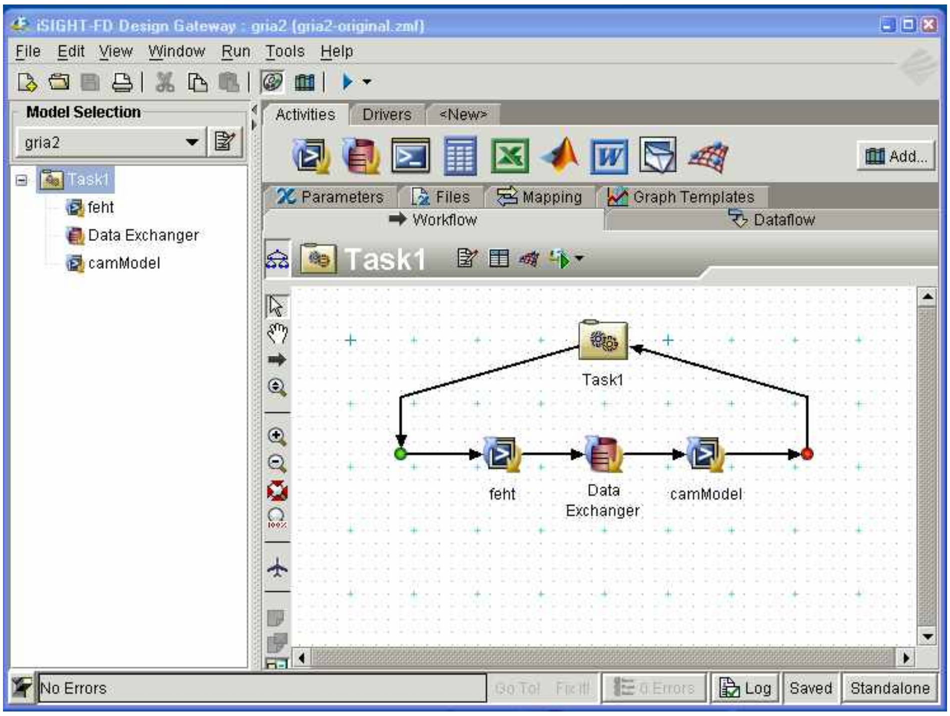

Figure 4: iSight-FD® TPM (local FEHT execution)

2.5.2 Phase II – Local MARC execution

For the purposes of the demonstration, Corus chose to replace the in-house FEHT application with the commercial FEM code Marc (PC 32 bit version 2007r1), available from the SIMDAT partner MSC. However, rather than replacing FEHT immediately with a GRIA-enabled MARC component, it was first necessary to set up a local MARC execution step, in order to gain some experience of MARC itself, and to ensure that suitable output data could be obtained for an equivalent test case input file to that used by the FEHT solver. The resulting workflow is shown in Figure 5.

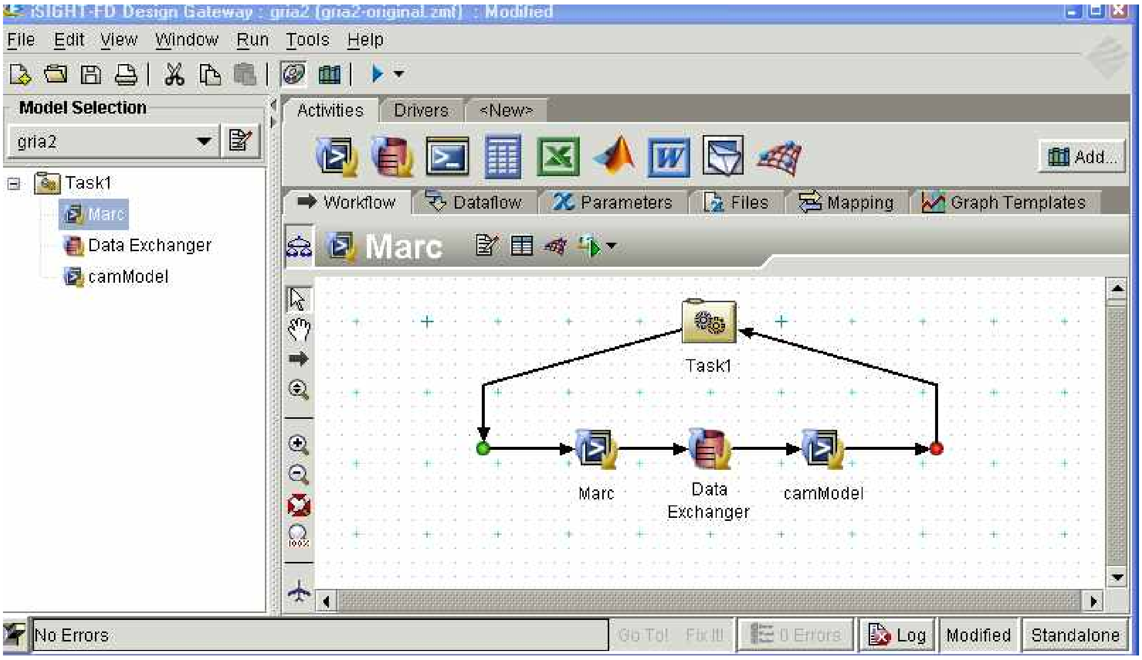

Figure 5: iSight-FD® TPM (local MARC execution)

2.5.3 Phase III – Remote MARC execution

The final phase of the set-up involved replacing the local MARC iSight-FD® component with one representing the remote execution of MARC via GRIA (see Figure 6). The component used was based on the GRIA plugin for iSight-FD®, from EADS.

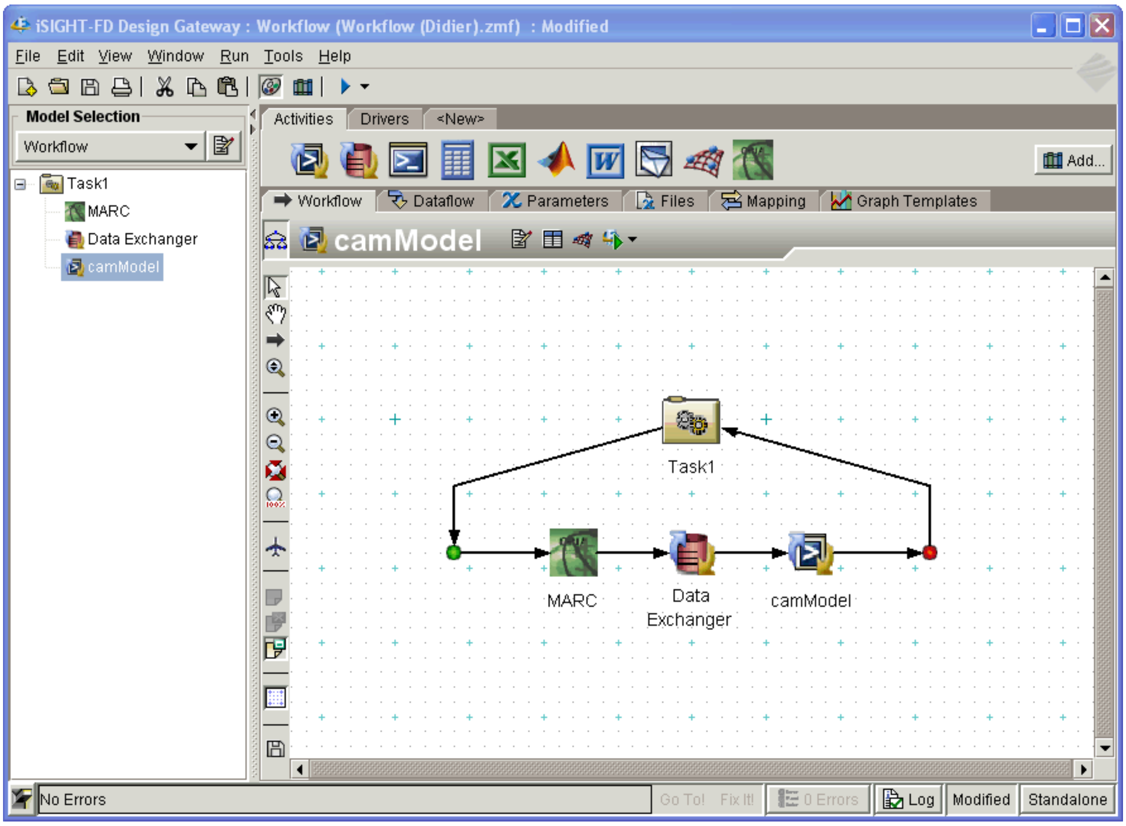

Figure 6: iSight-FD® TPM (remote MARC execution)

Once the component had been added to the workflow, it was simply a case of configuring this to:

- Specify a remote GRIA Job Service
- Select an appropriate Service Level Agreement (SLA)
- Select an application (i.e. MARC), as provided by the Job Service
- Configure the job inputs and outputs (e.g. specifying sources file for inputs and target files for outputs)

Figure 7 demonstrates the configuration of the GRIA component, as outlined above. Here we select the GRIA Job Service at Fraunhofer as the service provider. The SLA is called "MARC (new)", which has been negotiated previously (using a GRIA client). The "MarcTemperatures" application service is then selected (see Chapter 6). Job inputs are configured to originate from local files and similarly for the outputs. Finally, no specific application arguments are necessary here.

The final part of the configuration for the MARC job is to define the actual source input files and destination output files (see Figure 8 and Figure 9).

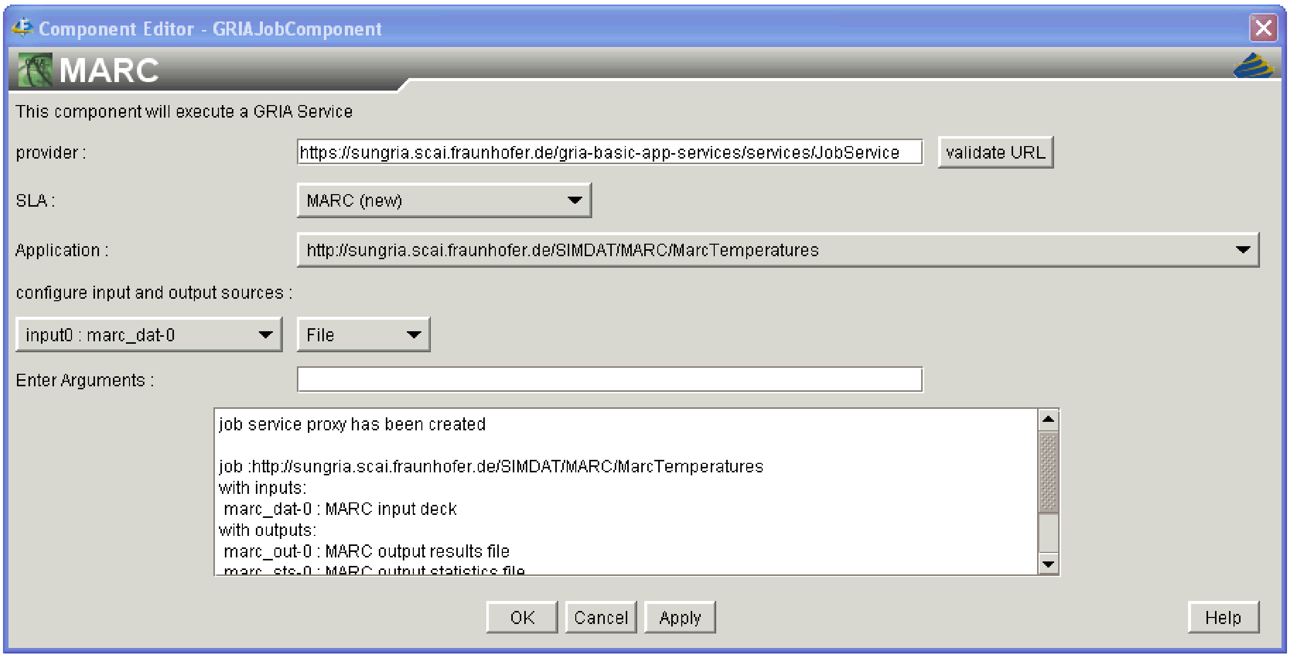

Figure 7: Configuration of MARC job using GRIA plugin for iSight-FD®

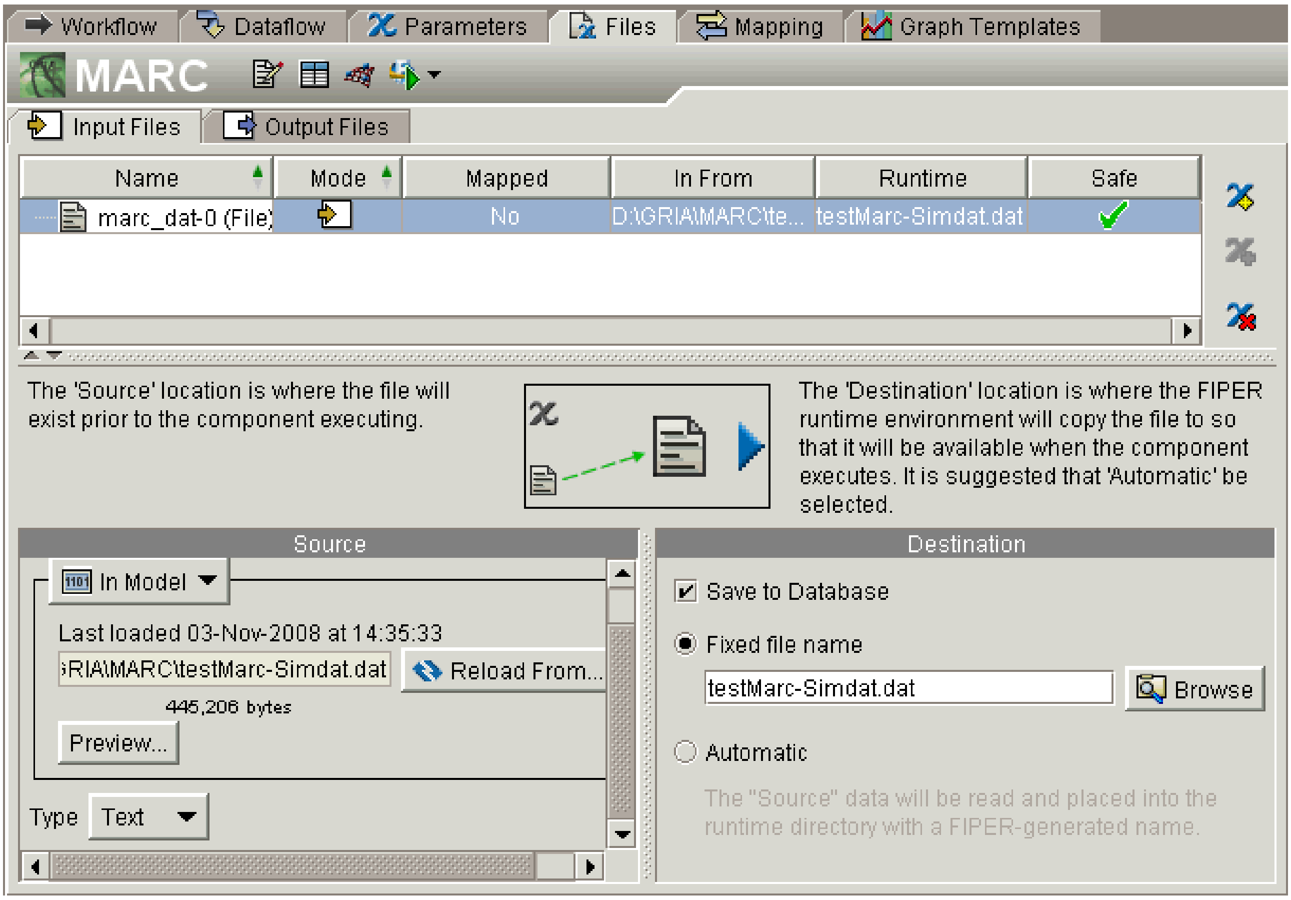

Figure 8: Mapping of inputs for MARC job, using GRIA plugin for iSight-FD®

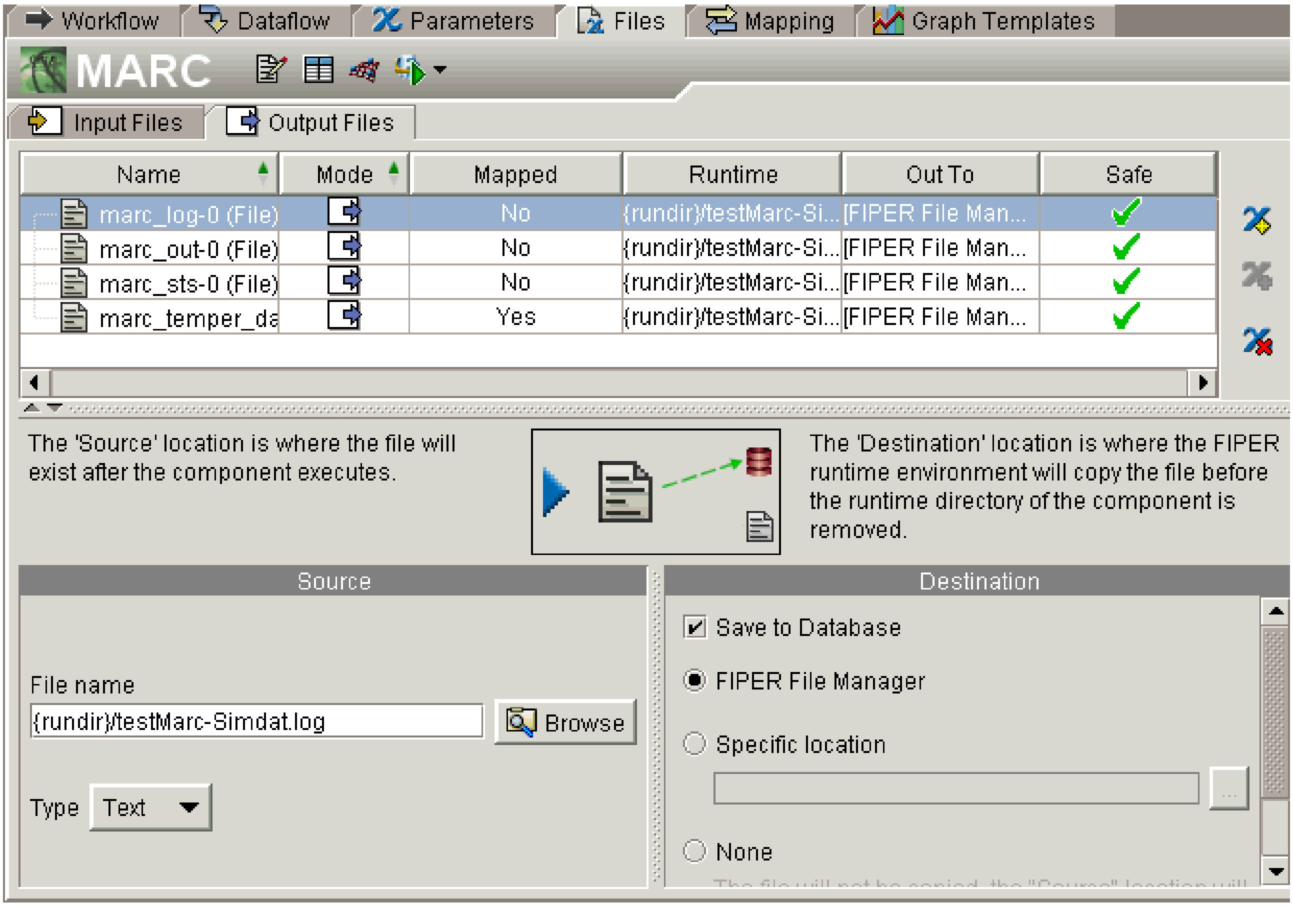

Figure 9: Mapping of outputs for MARC job, using GRIA plugin for iSight-FD®

3 SIMDAT Technology

The SIMDAT Grid Solution Portfolio has been developed to meet the needs of industrial partners undertaking the collaborative design of complex products in four application sections; aerospace, automotive, meteorology and pharmaceutical. The portfolio consists of Grid technologies supporting both infrastructure (security, management, discovery, data access, execution and workflow) and application (problem solving environments and analysis tools) capabilities. The portfolio has been designed using a service-oriented architecture based on key web service and Grid interoperability specifications. The Grid technologies within the portfolio are provided from a variety of vendors. The majority of technologies are developed by SIMDAT partners whilst some are supplied by 3rd party organisations external to the project, where additional important capabilities have been identified. Many SIMDAT partners offer technology on commercial terms whilst some partners use an open source distribution strategy to ensure a wide adoption of technology.

The following sections outline the SIMDAT technologies used within the Corus demonstrator.

3.1 Integrated Grid infrastructure: GRIA

GRIA (www.gria.org) is a service-oriented infrastructure designed to support Business to Business (B2B) collaborations through service provision across organisational boundaries in a secure, interoperable and flexible manner. GRIA makes use of business models, processes and semantics to allow service providers and users to discover each other and negotiate terms for access to high-value IT assets. By focusing on business processes and the associated semantics, GRIA enables users to provision for their computational needs more cost effectively, and develop new business models for their services.

3.2 iSight-FD / GRIA plug-ins

The problem solving environment, iSight-FD®, is already used by Corus to integrate various applications as workflows. iSight-FD® provides an API to enable plug-ins to be written for new applications. This feature has been exploited by EADS, who has already written a plug-in for GRIA, as part of the SIMDAT aerospace activity.

The GRIA plug-in adopts the common interfaces provided by other wrapped applications, but also acts as a GRIA client, orchestrating any necessary interactions with GRIA services in order to define a GRIA job and to execute it. Any remote GRIA Job Service may be configured for use, simply by entering its endpoint URL. Support for managed services is also provided. For example, if a user is required to present a valid SLA to the Job Service, a list of the user's SLAs is presented as a drop-down list.

Via a single GRIA plug-in, the iSight-FD® user can access any application that has been deployed on a GRIA Job Service.

3.3 MSC Marc

Finite element analysis (FEA) is a critical part of the virtual design process. As a non-linear FEA program, Marc enables an engineer to assess the structural integrity and performance of parts undergoing large permanent deformations as a result of thermal or structural loading. The types of deformations the program can study include geometric nonlinearities (metals bending) and material nonlinearities (elastomers and metals that yield under structural or thermal loading). One can also use Marc to simulate deformable, part-to-part or part-to-self contact under varying conditions that include the effects of friction—critical for analyzing nonlinear behaviour in tool-and-die set-up, spring coil clash, or a windshield wiper system.

Whether one is designing with glass, rubber, steel, or concrete, Marc offers an extensive library of metallic and non-metallic material models, along with a library of 175 elements for structural, thermal, and fluid analysis.

MSC are already a Corus supplier and Corus are familiar with their products such as MSC Marc.

4 Customers and Service Providers

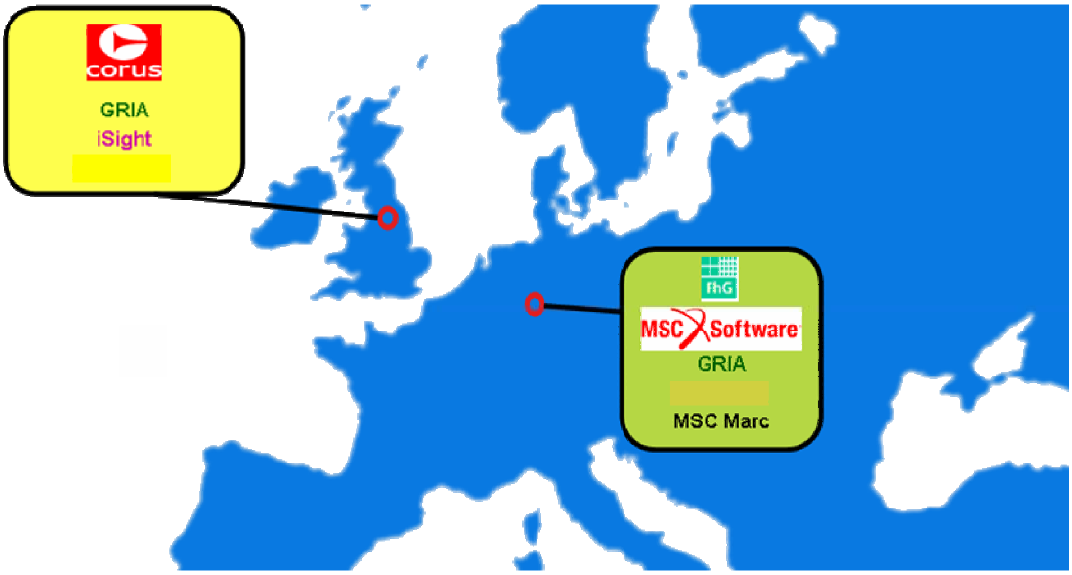

Figure 10: Customer and Service Provider

Figure 10 shows the deployment scenario for the Corus demonstrator. The following sections describe the customer and supplier deployment in more detail.

4.1 Customer (Corus)

Corus are the customer in this scenario. They already use the iSight-FD® PSE (from Engineous), which facilitates the use of various wrapped applications. For the demonstrator, we installed the GRIA plug-in for iSight-FD® (from EADS), providing GRIA client functionality in a "GRIA" component, which may then be added as an application step into any iSight-FD® workflow. Corus steel engineers then had the option to use applications located at Corus, or at remote analysis service provider sites.

4.2 Service Provider (FhG)

FhG were already operating a GRIA service provider for other SIMDAT demonstrations, so could therefore act as an application (and computational resource) provider for the Corus demonstrator.

For the deployment, FhG carried out the following steps:

1. Installed MSC Marc (PC 32 bit version 2007r1) on FhG host.

2. Tested Marc as standalone application.

3. Developed MARC application wrapper for GRIA (startJob.pl), plus metadata describing the application.

4. Deployed MARC wrapper and metadata, creating a new MARC application service for GRIA.

The service was tested initially, using standard GRIA clients, both at FhG and IT Innovation, before being tested by Corus, via iSight-FD®.

5 Key innovations

The key innovation for Corus was to be able to transparently outsource analysis services in their iSight-FD® workflows to a 3rd party service provider of their choice.

The GRIA plug-in for iSight-FD® hides the business negotiations that take place between accountable managers by using policies (Service Level Agreements) enforced by the GRIA middleware, allowing engineers to concentrate on their results.

6 Challenges Overcome

The Corus demonstration did not require any further developments of the Grid infrastructure (GRIA), however a number of issues were raised w.r.t. the integration with iSight-FD® and the development of the MARC application service. These are discussed below.

MARC provides support for the runtime compilation of user-supplied FORTRAN subroutines. This feature was required by Corus to enable MARC to output the temperatures file required for the subsequent step in their workflow. The difficulty here is that, if a user supplies his/her own code fragments to a service such as this, there is no guarantee that the resulting job will work. For example, the FORTRAN may need to refer to various system libraries, and there is no way that a client "developer" can know this information a priori. There are also security concerns in allowing arbitrary code to be uploaded to a service. For this reason, we decided to create a new "MARC-Temperatures" service, in addition to the standard application, which was already configured with the necessary FORTRAN code in order to create the temperatures file, which could then be published as a formal output (data stager) of the MARC application.

The MARC service seemed to be suffering from some reliability problems, when tested more intensively by Corus. Some jobs randomly failed and were destroyed, with nothing being reported to the client, via the iSight-FD® plug-in. This was eventually discovered to be due to a combination of slightly restrictive constraint in the MARC SLA (number of CPUs <= 1 CPU) and a known bug in the GRIA 5.2 SLA Service (causing the current value of the CPU count to be miscalculated, e.g. 1.00046 instead of 1). This bug has been fixed in GRIA 5.3 but we were not in a position to upgrade the GRIA services at Fraunhofer. To overcome this issue, the SLA constraint was relaxed, with subsequent tests showing 0 job failures out of 30 submitted.

Finally, the MARC software on the Fraunhofer host was only configured for one license and therefore the analysis service could not support concurrent users. In practice, a commercial service provider would normally provide multiple licenses, and a more sophisticated means of provisioning jobs according to available licenses, as demonstrated by the automotive prototype with ESI[1].

The iSight-FD® plug-in from EADS required minor bug fixes and enhancements. The plug-in was written as a prototype by EADS, and had not undergone quality assurance beyond the requirements of initial aerospace prototypes earlier in SIMDAT. In addition, IT Innovation was not in a position to test iSight-FD® with the GRIA plug-ins, as no license was available for iSight-FD®. Therefore, only limited bug fixing and enhancements could be made for this demonstration.

The plug-ins were developed for GRIA 5.1 and needed to be updated for GRIA 5.2. The upgrade ensured that new SIMDAT features could be supported such as JSDL support, named inputs/outputs, optional inputs and arrays. We could not upgrade to GRIA 5.3 because this would

[1] D.9.3.2: Documentation of Final Implementation of SIMDAT Automotive Prototypes

require a more extensive re-write of the plug-in, due to extensive refactoring of the APIs from 5.2 to 5.3. Whilst the plug-in did provide a simple interface for authoring workflows that include 3rd party analysis services, there were some usability concerns. For example, the action of editing a GRIA job configuration reset all current configurations for that job. Also, Corus found that it was not possible to display the current configuration after closing and re-opening a workflow. This made it impossible to see which service provider or which GRIA application was being used for a job. At the time of writing, this issue remains to be fixed.

7 Benefits

The collaborative nature of Corus's RD&T business is ideally suited to SIMDAT's objectives and the capabilities of the SIMDAT Grid Solution portfolio are aligned with both business and technological needs. Corus RD&T has a policy of collaborative product development with key customers in its principal markets with a strong emphasis on developing high added value products. Corus also works with research institutes around the world in order to develop cutting-edge, innovative technologies. Corus RD&T use the latest modelling and simulation methods in the design, development and selection of steel chemical compositions, mechanical properties and processing for optimum performance in steel product manufacturing. The design processes use similar techniques to other SIMDAT engineering disciplines such as design optimisation algorithms, finite element modelling and through process modelling although the scenario focuses on upstream steel modelling and manufacturing rather than the development of downstream products (cars, aeroplanes, etc). Corus are experienced in using workflow environments as a way of representing complex scientific processes and have recently selected iSight-FD® after detailed evaluation of other competitive platforms (e,g. Model Center). Isight-FD® now replaces their previous Steel Modelling Workbench developed under European funding. Both of the commercial TPM Workbench technologies are deployed within SIMDAT and form part of the solution portfolio.

To support the development of the demonstration SIMDAT partners have provided Corus with training and support, helping Corus to understand how Grid technology can support collaborative product design and how such technologies can be deployed within their business.

Corus can benefit through collaboration with SIMDAT in many ways. SIMDAT is a successful European project that is delivering Grid solutions to industry today. The technology offering is based on commercial and open source products rather than research prototype software and therefore most of the solutions have been industrially hardened at this stage. In addition, SIMDAT application and technology partners have extensive experience in developing and deploying service-oriented infrastructures that can support inter-domain business partnerships, a core part of Corus's business. Corus has been given access to software from the Grid Solution portfolio necessary to build a demonstration prototype and access to technology experts, providing consultancy on how Corus can utilize the Grid to integrate design engineers into their customers' supply chain. The use of Grid technologies for collaborative product design allows Corus to:

- share design specifications and performance data required to support the collaboration in a controlled and managed way;
- procure software services and computation from service providers in a way that is optimised to the demands of their engineers; and
- inject quickly new innovative analysis capabilities and experts into their design processes.

By making use of spare, in-house, computational resources, Corus can make significant savings on the cost of procurement. By using out-sourced resources, Corus can avoid needing to buy costly, high-performance computing resources, which depreciate quickly but also gain potential access to software codes for specific/targeted applications. Furthermore, the increase in speed of out-sourced calculations reduces the turnaround time for simulations, improving the time-to-market of new products.

8 Best Practice and Lessons Learned

A GRIA Job Service often exposes a number of applications. Each application has a pre-defined set of input and output data stagers along with some defined application arguments (as defined in the application metadata). Sometimes, an argument value can affect the actual number of outputs produced for a job (for example, if a data stager is defined as an array of outputs of a certain type). In addition, an output data stager may sometimes be filled with empty data. Complex applications (such as MARC) can be executed in many different ways, due to the many parameters available, in order to cater for a wide range of executing conditions. Clearly, there is a high risk that certain combinations of parameters or particular parameter settings will result in job failures, which can be very difficult to troubleshoot. Therefore, "ambitious" designs of applications should be discouraged. We therefore suggest that a Job Service always exposes applications with the least degree of freedom necessary to execute an application reliably and reproducibly.

This point is of even more concern when using a GRIA application as part of a workflow. These applications should be highly constrained, i.e. having a well-defined number of inputs/outputs, such that these can be built into workflows. This is one reason why, in our demo, we ended up creating a tailored MARC service to always output temperatures, and NOT allow the user to provide arbitrary FORTRAN code (see discussion in Chapter 6).

A GRIA user identity is currently stored in a local keystore, with its password stored in a crypto.properties file in plain text. The user should be made aware that his/her local keystore and password should be kept securely in order to prevent identity theft. This concern was addressed in GRIA 5.3 which no longer requires the use the Axis crypto.properties file.

Error messages related to an SLA should be made clear. For example, it makes more sense to prompt the user with a contact telephone number of the service provider when he/she has exceeded his/her CPU usage, rather than saying the user is not authorized to perform a particular job. Some more constructive feedback or suggestions about what to do to rectify the situation would be helpful. This is even more critical when an application is part of a workflow, as there may be many steps to finish successfully in order to complete the workflow. The user should have more control over whether a job “fails” due to violated constraints, or simply gets charged more for the additional usage, for example.

9 Conclusions

Corus has successfully tested the benefits of using SIMDAT GRIA services centred around Workbench technology thus providing a means for easy internal deployment of distributed services as well as allowing access to out-sourced resources. This will certainly provide both technical and commercial benefits to Corus over commercial services such as FIPER from Simulia. It is therefore recommended to test initially within RD&T the GRIA services with/without iSight-FD plugins internally prior to carrying out feasibility studies with Business Units and Tata Group. In parallel, applicability of such technology with Academia such as Sheffield IMMPETUS will be explored. Development in collaboration with IT Innovation and EADS for an ABAQUS/ISIGHT FD® plugin should be explored for maximising technical and commercial benefits of using and deploying such technologies for product and process design and simulation. It remains to be seen, however, if ISV software vendors will be prepared to embrace such concepts for code evaluation or providing services on demand. Further development of GRIA services and applications should target the FEM Code ABAQUS which will increase usability and applicability for process and product design within the UK.