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

Deliverable

D3.1.1. Consolidated requirements report and SIMDAT
Distributed Data Repository Access design

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1 Introduction

1.1 Purpose

This document represents the public version of the deliverable D3.1.1 WP3 Consolidated requirements report and SIMDAT Distributed Data Repository Access design of SIMDAT in the Integrated Project IST-2002-511438.

The document presents consolidated specification of the SIMDAT distributed data repository access requirements as derived from state-of-the-art analysis and requirements discussions with SIMDAT application sectors and technology activities. The purpose of this deliverable is to provide a public version of the detailed goals of WP3 distributed data repository access. The document states what the software will do and also proposes a high-level architecture defining the scope of distributed data repository access in reference to other technology activities.

SIMDAT partners (stakeholders) have a diverse range of expertise representing both application sectors and horizontal technology activities. The document is structured to give a view of distributed data repository access from each application and technological stakeholders’ perspective.

1.2 Scope

Modern commercial processes deployed to manage the design, development and production of products - whether these are automobiles, aircraft, drugs, or services such as meteorology - are highly complex. In every case these processes are further complicated by external factors. Such factors include increasingly stringent regulatory environments and the commercial pressure to collaborate in order to share (or mitigate) technical and/or financial risk. The challenge for SIMDAT is to develop and deploy technology and techniques that will improve the ability of organizations to collaborate in a flexible and dynamic fashion. This collaboration is required at a deep technical level, with applications, databases and resources talking directly to one another in a controlled and secure fashion.

The complex problems to be solved all involve multiple data repositories describing aspects of the product and process development. Typically in different departments and at different

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1 SIMDAT Annex I
sites, these are currently not directly linked with each other. The Pharmaceutical sector is most advanced in integrating data repositories. Tools like SRS from LION or Discovery Link from IBM allow different databases and flat files to be interlinked. However, these data repositories need to be available at a common location. Therefore copies of remote data repositories are exchanged and updated periodically. In other industrial sectors like the automotive and aerospace industries, concepts for interlinking these different distributed data repositories did not exist prior to the start of the SIMDAT project.

Design of many products is essentially multidisciplinary, involving the solution of complex problems which are correlated with each other. Minimizing the risk of injury to a pedestrian in a car accident conflicts with the mechanical stability of the bonnet, and a compromise has to be found. The designer of one subsystem needs to know about the design changes of other development teams, to get direct access to simulation results of other disciplines and to get seamless access to simulation methods for all disciplines in order to successfully apply multidisciplinary optimization tools.

Correlation of data generated in different departments or at different sites within a global organization is a key problem for all industries represented in SIMDAT. Its solution requires distributed data access with a clear definition of the semantics of the databases involved, and enables the retrieval of relevant information even though it might not be simply represented in any single database. Integration through a data Grid requires not only basic mapping of semantics between the major data repositories involved but also brokering of applications that serve analysis and mining procedures. Dynamic object assembly will be necessary to create new objects that are compliant with data mining and data analysis tools. Special attention must be paid to security, e.g. where third-party suppliers have need-to-know access to data and correlation may provide insight into confidential processes.

Knowledge services will add enormous value to virtual data repositories. Using knowledge discovery tools on a virtual repository containing all details of a design process creates the opportunity to extract and formalize successful strategies for design improvement.

The strategic objectives of SIMDAT are:
- to test and enhance Data Grid technology for product development and production process design,
- to develop federated versions of problem-solving environments by leveraging enhanced Grid services,
- to exploit Data Grids as a basis for distributed knowledge discovery,
- to promote de facto standards for these enhanced Grid technologies across a range of disciplines and sectors, and
- to raise awareness for the advantages of Data Grids in important industrial sectors.

Four application sectors have been selected to cover the full range of issues to be addressed in design, development and production of complex products and services: the aerospace, automotive and pharmaceutical industries, and meteorology. For each sector complex problems have been identified as use-cases for the project.

Seven key technology layers have been identified as important to achieving the SIMDAT objectives:

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- an integrated Grid infrastructure, offering basic services to applications and higher-level layers;
- transparent access to data repositories on remote Grid sites;
- management of Virtual Organizations;
- scientific workflow;
- ontologies;
- integration of analysis services; and
- knowledge services.

### 1.3 Definitions, acronyms and abbreviations

DAIS: database access and integration services

FTP: file transfer protocol

GGF: global Grid forum

GRIA: Grid Resources for Industrial Applications

HPC: high performance computing

OGSA-DAI: open Grid services architecture – database access and integration

OGSI: open Grid services infrastructure

RDBMS: relational database management system

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

UNICORE: uniform access to computing resources

VO: virtual organisation

WS-I: web service interoperability

WSRF: web services resource framework

XML: extended markup language
2 Overview

Data repositories are key to the design, development, and production of complex products and services. Different data repositories store product design data, results from physical tests, and numerical simulation results characterizing the functional properties of products and processes, as well as knowledge about the design process itself, material properties and development strategies. These data repositories might be a collection of (relational) data bases and/or a collection of flat files.

Distributed and collaborative development is day-to-day practise in product and process design. Multinational companies operate worldwide networks of specialized development centres, focusing on different aspects of development tasks. Consultants and component providers support the development processes. At each development site different departments have to collaborate with each other. However, currently there is a reliance on peer-to-peer translation systems that are specifically developed for each individual set of interactions. This is expensive and time-consuming, and there is a pressing need for more automated and standardized methods to manage site-to-site data flows.

SIMDAT focuses on the data aspects of Grids, in particular on the federation of databases across sites involving different data representations and formats. Up to now in Grid projects, questions of data access and federation have been addressed in a limited way, with basic data transfer (e.g. GridFTP) and data cataloguing and replication (provided e.g. by the European Data Grid project). However, basic support for accessing remote databases has been developed in the UK e-science project OGSA-DAI. Deployment issues have been largely neglected, making the setup and management of Grids difficult, preventing major uptake in commerce and industry.

2.1.1 Access to distributed data repositories

Web service-based interfaces to remote and distributed databases have been developed for a long time, and the majority of web service applications actually rely on such functionality. The Grid community has originated from the high performance computing (HPC) activities, and this heritage shows in the emphasis on sharing computational resources (i.e. CPU cycles) readily apparent with current Grid systems. Data issues have mostly been addressed on the level of transmitting files or data streams (GridFTP, UNICORE file streaming).

The emergence of web service related interface standards (OGSI; WSRF) and the needs of applications (UK e-science, CERN LHC) have led to the development of prototypical support for data federation. The OGSA-DAI project3 (Open Grid Services Architecture - Data Access and Integration) within the UK e-science Core Programme has proposed a Grid service interface for read access to remote databases and for distributed queries. A reference implementation working with the Globus Toolkit is available, and work is underway to support the upcoming Globus 4 and other WSRF-compliant Grid systems, and to provide a pure web services interface. A WS-I compliant version is available. In the European Data Grid project components for the management of data catalogues and replicas have been developed. In the first phase of SIMDAT focus is towards integrating these components into a comprehensive data access layer based on web services and hardening/extending it to match the requirements of the application activities.

Based on the state-of-the-art, and in close cooperation with other ongoing Grid projects SIMDAT enhances existing software environments regarding distributed data repository

access to support industrial needs, in particular to support access and remote updates of remote data bases using Grid services.

As one of the common denominators of the SIMDAT application clusters, access to data that is residing on a remote Grid node or that is distributed across many Grid nodes is required. On top of the access functionality, higher level services like coordinated distributed queries, support for semantic interoperability based on ontologies etc. will be built in the application activities and in the technology components. The access services to be developed in this component will over the full duration of SIMDAT offer the following functionality:

- Provide transport (across different underlying database implementations) access to databases residing on local or remote Grid nodes, supporting a full set of query and database access functions. Distributed read access from n readers will be supported, with distributed write and/or update being developed in close cooperation with the application activities that need them (in particular, the automotive applications).
- Offer middleware-level functionality for coordinated distributed queries spanning a number of database instances across multiple Grid nodes, interfacing with the workflow technology component.
- Allow transparent access to files that are indexed using a database, plus directory services for same. There is no need for presenting a consistent global file system view across multiple reference databases.
- Support attaching metadata and annotations to records that are sufficient for the intended use of provenance data, ontologies and knowledge discover/mining techniques in the respective technology component and application activities.
- Introduce fine-grain access control (up to the level of records) that can be tied in with virtual organisation (VO) functionality to finely express access and inspection rights for individuals according to their role in a VO (need to know), and for applications according to their requirements (e.g. a crash simulation needs to be able to access data that may be otherwise unreadable by a VO participant).
- Allow the introduction of caching and replication mechanisms in a way transparent to the end-user to improve performance, with actual implementation of such mechanisms being done in the application activities that have demanding performance requirements.

From the ongoing analysis, it is clear that distributed read and initial update functionality (from first topic), basic distributed query functionality (second, third, and fourth topic) and initial support for caching and replication (fifth topic) will be needed for the PM 12 demonstrators.

Ensuring swift progress, first releases of the data access services are being derived from existing work. It is proposed to extend the functionality of these components to accommodate the application activities. Currently the primary candidate for distributed data access components is the result of the OGSA-DAI project\(^4\). OGSA-DAI has specified a Grid service interface for accessing data bases across OGSA compliant Grid systems on Grid nodes and developed a reference implementation covering important data base engines (IBM DB2, Oracle, …). On top of the basic access services, support is available for service composition and (in a prototype form) distributed queries. The reference implementation has been integrated with Globus Toolkit and is available as open source. Work to integrate with other OGSA-compliant Grid systems (especially GRIA\(^5\), see below) is under way, as is provision of a pure web service front end to the OGSA-DAI functionality. Standardization of the data

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\(^4\) [http://www.ogsadai.org.uk](http://www.ogsadai.org.uk)

\(^5\) [www.gria.org](http://www.gria.org)
access interfaces within the OGSA-DAI working group of the GGF is progressing. Planned releases in time for the final demonstrator of SIMDAT include the implementation of a WSRF interface possibly with integration with Globus Toolkit.

A suitable data access layer integrated with the Grid infrastructure prototype will be made available to the SIMDAT partners in the upcoming months. After transitioning from initial (possibly proprietary) data access platforms, the application activities will be able to rely on the basic data access services available thus. The work in these areas will benefit from having a stable platform and getting support during installation and operation. Emphasis is being put on portability and interoperability by relying on de-facto standard interfaces, thereby protecting the SIMDAT developers’ and users’ investments.
3 Overall Description

Over the past 20 years relational database management systems (RDBMS) have evolved to provide reliable and scaleable solutions for data management. Most of today’s enterprise applications rely on RDBMS technology to provide effective storage of and access to application data. The propagation, throughout the enterprise, of disparate databases and their dependant applications has created an environment where applications operate in isolation and have difficulty interoperating.

Typically, a business process would include many heterogeneous applications operating on business objects derived from disparate databases distributed within an organisation or even inter-organisation. The traditional approach to overcome data integration issues within an organisation is to develop a single data warehouse for the enterprise that integrates with all applications involved within its business processes. The reality however is that this is not always possible because either the applications are controlled by multiple vendors or they are operated by external organisations with different IT strategies.

An alternative approach is to provide federation between heterogeneous databases. High-end solutions such as DB2 and Oracle provide federation using distributed queries across disparate databases with the same or different schemas. Similarly, the OGSA-DAI working group are developing a generic web service that provides distributed query processing between different databases. However, the distributed query protocol is in its early stages and will not be available until next year.

Federation at the database level operates on table data, which may not be appropriate for the exchange of data between tasks in a business process. For example, a business process may operate on higher-level business objects that are derived from underlying databases; in this case application level federation may be more suitable.

3.1 DAIS and OGSA-DAI

3.1.1 DAIS

DAIS\(^7\) is the Database Access and Integration Services Working Group within the Global Grid Forum (GGF). The group was established following a Birds-of-a-Feather session held at GGF4 in February 2002. It seeks to promote OGSA compliant standards for Grid database services, initially focusing on providing consistent access to existing, autonomously managed databases. It does not seek to develop new data storage systems, but rather to make such systems more readily usable individually or collectively within a Grid framework.

3.1.2 OGSA-DAI

OGSA-DAI is a collaborative programme of work involving the Universities of Edinburgh, Manchester and Newcastle, with industrial participation by IBM and Oracle. Its principal objective is to produce open source database access and integration middleware which meets the needs of the UK e-Science community for developing Grid and Grid related applications. Its scope includes the definition and development of generic Grid data services providing access to and integration of data held in relational database management systems, as well as semi-structured data held in XML repositories. The current phase of work began in October 2003 and is scheduled to develop higher-level database access and integration services by September 2005.

\(^6\) [http://www.ogsadai.org.uk](http://www.ogsadai.org.uk)

\(^7\) [http://www.Gridforum.org/6_DATA/dais.htm](http://www.Gridforum.org/6_DATA/dais.htm)
OGSA-DAI also represents a significant contribution on behalf of the UK e-Science Core Programme to extend the Grid model to include database interoperability. OGSA-DAI works closely with DAIS and it is intended that the software will serve as a reference implementation for DAIS standards.

3.1.3 OGSA-DAI compliancy with DAIS standard recommendations

Ultimately, OGSA-DAI software must be fully compliant with the DAIS Grid database service in order to become a reference implementation for the first version of a standards recommendation. However it will not always be possible to keep OGSA-DAI and DAIS fully synchronised in terms of their functional scope and interfaces during their respective developments. There are two reasons for this:

The Grid database service must be compliant with OGSA-based Grid standards and is dependent on related emerging Web Services standards, which are currently being fixed. OGSA-DAI is somewhat dependent on evolving Globus Toolkit software, itself a reference implementation of the Grid service specification. Consequently, not all software interfaces are under the control of the OGSA-DAI team. In addition, the OGSA-DAI development is being used to validate the emerging DAIS conceptual model, functional specification, and Grid database specific interfaces. Therefore to some degree, DAIS and OGSA-DAI activities are driving each other. The OGSA-DAI will use best endeavours to minimise the points of synchronisation between the DAIS specification definition and the OGSA-DAI software to minimise disruption to the growing number of OGSA-DAI users.

Further information on the GGF and DAIS are available from:
- DAIS Working Group\(^8\)
- Global Grid Forum\(^9\)

3.2 Functions

OGSA-DAI is a middleware product which supports the exposure of data resources, such as relational or XML databases, on to Grids.

OGSA-DAI is motivated by the need to:
- Provide an extensible framework for easily integrating data resources on to Grids.
- Allow metadata and the data resources in which they are stored to be obtained.
- Provide a framework to facilitate the discovery of data that may be distributed, or replicated, over many different types of data resources, the locations of which may not be known beforehand.
- Allow different types of data models, e.g. XML, relational or files, from distributed data resources to be easily integrated to Grid applications.
- Allow services to be discovered that provide access to data resources holding required data.
- Allow data to be accessed through uniform interfaces.
- Facilitate the integration of data from various sources to obtain the required information.

OGSA-DAI provides an extensible framework that allows access to and updating of data resources. Inherent data resource capabilities may be exploited and exposed to the Grid, such as performing SQL queries or XPath statements on data, as well as providing additional data manipulation functionality, such as asynchronous delivery or data transformation, that

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operates at the service layer. Using the OGSA-DAI interfaces disparate, heterogeneous data resources may be accessed in a uniform manner. It is important to note though that the underlying data model is not hidden - a relational data resource remains a relational resource and will not masquerade as an XML data resource unless that mode of access is already supported by that data resource nor does OGSA-DAI provide a query language that is not already supported by the data resource or through some other third party application.

OGSA-DAI exposes data resources through services. Clients interact indirectly with data resources via these services. OGSA-DAI provides services compliant with the popular Web and Grid services specifications:

- Web Services Interoperability (WS-I)\textsuperscript{10}
- Web Services Resource Framework (WS-RF)\textsuperscript{11}

OGSA-DAI services can be used as the basic primitives for creating sophisticated higher-level services that offer capabilities such as data federation and distributed query processing. The OGSA-DAI middleware layer can abstract away concerns such as database driver technology, data formatting techniques and delivery mechanisms, etc from these higher-level services.

OGSA-DAI is intended to contribute to a future in which, it is envisaged, scientists and engineers will move away from technical issues such as handling data location, data structure, data transfer and integration and instead focus on application-specific data analysis and processing.

### 3.3 Other distributed data management possibilities researched

Other possibilities for distributed data access and integration have been researched and evaluated as well. Among those are the established Grid data transfer/access tools:

- LHC and EGEE data management – CERN
- SRB (storage resource broker) – SDSC
- NERC data Grid

As well proprietary solutions are available but need to be licensed:

- Avaki global shared file system
- IBM DB2 information integrator etc.
- Oracle 10g, 11i, ...

Due to reasoning similar to the last paragraphs it is most useful to use OGSA-DAI as much as possible and concentrate effort on that.

For a brief overview of these data transfer/access tools please refer to the following paragraphs.

#### 3.3.1 LHC/EGEE data management

The Enabling Grids for E-sciencE (EGEE\textsuperscript{12}) project is funded by the European Commission and aims to build on recent advances in grid technology and to develop a service Grid infrastructure which is available to scientists 24 hours-a-day. Data management in the EGEE context has three major parts:

- Storage management
- Data catalogs

\textsuperscript{10} [http://www.ws-i.org/](http://www.ws-i.org/)


\textsuperscript{12} [http://public.eu-egee.org/](http://public.eu-egee.org/)
Transfer scheduling

In the gLite middleware stack, the data management functionality is provided by a set of services. The design of these services is driven by the principles of interoperability, portability, modularity and scalability. By using Web Services and a Service Oriented Architecture approach where each service interface is described by a Web Service Description Language document, they assure that the first two principles are met.

Initially for the gLite data management stack they make the assumption that the lowest granularity of the data is on the file level. They deal mostly with files if it comes to application data as opposed to e.g. data sets, data objects or tables in a relational database. The reason for this arguably very restrictive assumption is twofold: Most importantly, the initial two application groups to work with gLite are the High Energy Physics and Biomedical communities, for whom data are stored mostly in files. The second reason is that the semantics of files are very well understood by everyone, both on the service provider and application side, which is not the case for generic data objects for example, where every application group has their own definition thereof. For gLite to solve a generic problem they start with a semantically well-understood system, hence the choice to start solving the Grid data management problem for files, building on the work of previous projects, most notably the EU DataGrid and AliEn.

In order to not to have to deal with the peculiarities of each individual storage, it is required that all Grid-aware storage is implemented along the Storage Resource Manager (SRM\textsuperscript{13}) interface which provides most of the functionality needed. gLite provides a lightweight SRM that can be put on top of a simple disk-based storage. The SRM interface itself is being standardized through the Global Grid Forum.

The end-user application only needs to use the gLite-I/O API in order to access its data - the storage back-end, the SRM and security services are used indirectly. The detailed semantics of file access will be different depending what kind of storage back-end is being used beneath an SE; there may be substantial latencies for reads and many more failure modes for write for some. Therefore the number of errors and messages is larger than for a conventional file system.

Another assumption made is that data is usually co-located (co-scheduled) with the application that needs it. In order to be able to do so, the Grid job scheduler needs to invoke the gLite Data Scheduler (DS) services in order to make sure that a given file is available at the chosen site where the job is to be run. This co-scheduling may not be always possible, so it may be necessary to access the data remotely - in which case the gLite-I/O will act as a proxy service. The Data Scheduling services will also expose all nontrivial interfaces to the user for data placement in a distributed environment.

To the user of the EGEE data services the abstraction that is being presented is that of a global file system, with very similar semantics. A client user application may look like a Unix shell (as in AliEn) which can seamlessly navigate in this virtual file system, listing files, changing directories, etc. The most important API is that of the gLite-I/O which enables user applications to open, read, write and seek through their files, using just the LFN or GUID as the file name to open the data. APIs for catalog manipulation (directory creation in LFN space, listing, etc.) are as well provide so that it is possible to interface the gLite data management functionality through a standard UNIX shell.

\textsuperscript{13} \url{http://sdm.lbl.gov/gsm/}

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3.3.2 SRB – storage resource broker

The San Diego Supercomputer Center (SDSC) at the University of California San Diego (UCSD) Storage Resource Broker (SRB\textsuperscript{14}) is client-server middleware that provides a uniform interface for connecting to heterogeneous data resources over a network and accessing replicated data sets. As the name implies, the Storage Resource Broker brokers storage resources. It provides access, via a uniform API, to various types of data storage across local and wide-area networks, and maintains meta-data about each stored object (files). SRB, in conjunction with MCAT, provides a means for accessing data objects and resources through querying their attributes instead of knowing their physical names and/or locations.

The SRB provides some of the abstraction mechanisms needed to implement data grids, digital libraries, and persistent archives for data sharing, data publication, and data preservation.

Storage resources can be directories in UNIX file systems, directories in Windows file systems, archival storage systems such as HPSS (and, previously, UniTree and DMF), binary large objects stored in a DBMS (DB2, Oracle, Illustra), database SQL-queriable objects in DB2 or Oracle, and tape library systems. Tape systems can be combined with disk cache into compound resources, and the SRB can function as a complete basic archival storage system. SRB includes a set of tape I/O functions and an interface to the STK tape library system.

SRB is not open source, although the source code is readily available to academic organizations and government agencies and commercial organizations are encouraged to evaluate and test it via a simple agreement. The normal distribution is via source. The UCSD business office wishes to maintain the SRB as proprietary and license it for commercial use and resale.\textsuperscript{15} General Atomics is commercializing a version that split from the SDSC version in 2001. This was SRB 1.1.8.\textsuperscript{16}

Apart from that, the biggest difference between commercial software and research products like the SRB is the lack of a quality assurance testing group. But the group claims to do a lot of testing of new features, as do collaborative sites. It is also a mature product as it has been in production use since 1997. In 2000, a government agency thoroughly examined the code and provided fixes (memory overruns, etc). The design is such that most problems are fail-safe, due the client/server design, and cross-checks within our MCAT library and of the DMBS systems themselves. SRB is built on the quality and robust-features of modern DBMSs.

3.3.3 NERC Data Grid

The British Atmospheric Data Centre (BADC)\textsuperscript{17} is the Natural Environment Research Council's (NERC) designated data centre for the atmospheric sciences. The role of the BADC is to assist UK atmospheric researchers to locate, access and interpret atmospheric data and to ensure the long-term integrity of atmospheric data produced by NERC projects. NERC Data Grid\textsuperscript{18} is a project lead by BADC and started in 2002 to build a grid which makes data discovery, delivery and use much easier, facilitating better use of the existing investment in the curation and maintenance of quality data archives. Further they intend to make the connection between data held in managed archives and data held by individual research groups seamless in such a way that the same tools can be used to compare and manipulate data from both sources. What NDG aims to achieve is the ability to compare and contrast data

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\textsuperscript{14} http://www.sdsc.edu/srb/
\textsuperscript{15} http://www.sdsc.edu/srb/srbOpenSource.html
\textsuperscript{16} http://www.nirvanastorage.com
\textsuperscript{17} http://badc.nerc.ac.uk/home/
\textsuperscript{18} http://ndg.badc.rl.ac.uk/
from an extensive range of (US, European, UK, NERC) datasets from within one specific context.

To reach those goals they strive to have a metadata model, storage and management, that support:

- incarnations for earth observation data
- based on digital library and industry standards
- many different flavours of metadata ...

Therefore there will be a distributed discovery mechanism and support for harvesting metadata as well as the possibility of separate discovery of and access to data.

Questions remain with respect to which storage systems can they interface to and which data transfer mechanisms they do support.

Version 0.1 of it can be downloaded.\(^\text{19}\) It contains source code and documentation for the NDG Version 0.1 release. While every effort has been made to make this a stable and functional release, the primary aim of this release is to make the work publicly available. As such this is an entirely unsupported release and there will be no technical support for this code offered by BADC (the NDG project lead) or other NDG partner organisations.

\(^{19}\) [http://ndg.badc.rl.ac.uk/downloads.htm](http://ndg.badc.rl.ac.uk/downloads.htm)
4 Specific Requirements for each application activity

4.1 Demonstrators

Requirements have been analysed for the following demonstrators which are planned for the end of the first year of the project.

- **Aero**: VO for collaborative multi-disciplinary (aeroacoustics, structural, aerodynamics) aerospace design
- **Auto1**: Federation Scenario showcasing
  - MSC.SimManager Federation
  - Data extraction from two MSC.SimManager data sources for data mining usage
  - Ontological integration of CAE and CAT databases
- **Auto2**: Optimus/GRIA integration for meta-scheduling on the Grid
- **Auto3**: VO for collaborative car design supporting confidentiality constraints of components between organisations
- **Meteo**: Meteorology portal that provides access to virtual meteorology database with supporting VO for access control
- **Pharma1**: SRS federation
- **Data Mining**: Technology demonstrator showing how data mining applications (WEKA) can be deployed within a Grid infrastructure
- **Ontological Integration**: Technology demonstrator showing how Ontobroker can be used to integrate local disparate data sources

For the contribution of each demonstrator towards the overall target of the SIMDAT project please refer to the application activity deliverables.
4.2 Aerospace

4.2.1 Overview

The aerospace industry deals with highly complex products that have data creation, management and curation requirements that span hundreds of collaborating organisations over a 50-year lifecycle. Partners on a product team need to collectively manage thousands of inter-related processes and this leads to expend considerable time and effort in the access, transmission, control, translation and sharing of data. The aerospace sector will develop and deploy existing and emerging Grid technologies and concepts to improve collaborative engineering of sophisticated products.

The development of aerospace products requires the collaboration of various engineering disciplines such as aeroacoustics and aerodynamics that are increasingly distributed within different organisations. Each discipline relies on a variety of commercial and bespoke in-house PSE’s and analysis tools to help solve complex design problems. The design models are complex and simulations are computationally expensive often executed on computational clusters accessed through batch submission systems such as PBS, Condor, etc. When designing a product engineers develop a dataflow that incorporates various analysis applications. The dataflow is used to explore a design space and hence find the optimum design solution. Typically today’s engineers codify these dataflows using scripts that read/write/translate data and execute local applications. Results are stored on the file systems and managed through a manual procedure.

A problem with this approach is that intra-enterprise collaboration is difficult and inter-enterprise collaboration is almost impossible within the constraints of most businesses. Collaborative engineering requires organisations and individuals to share resources within the constraints of their business. For example, if a script needs to execute an application on a machine provided by another organisation remote access has to be configured. This is difficult to maintain and usually involves systems administrators who may not be the right person to authorise access to the resource because they do not understand the business needs. If the application is not directly accessible collaboration across organisation boundaries has to be achieved using out-of-band distribution of data files. Network connectivity is usually over a secure VPN, which can be expensive.

Another problem is that aerospace dataflows is data formats and management. A typical dataflow may contain a diverse set of both proprietary and standard data formats. In some cases, engineers develop analysis codes that read and write data files in proprietary formats. Connecting two codes together requires both in-depth knowledge of the file formats and development of bespoke conversion utilities that are inherently difficult to reuse.

The aerospace sector is looking to define new business models that will demonstrate how engineers can collaborate more effectively across organisation boundaries. The initial scenario will 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. The scenario is one use-case selected from many possible alternatives in the product lifecycle that will be used as a “model problem” to drive the development and deployment of Grid technology.

A project manager working for a prime contractor initiates the business process by assembling a project team with the required core competencies to solve the design problem. The project
manager identifies engineers directly with the organisation responsible for co-ordinating the design and searches for service providers with an appropriate trust and Quality of Service credentials. The service providers advertise services and respect negotiated quality of service. The project team consists of engineers directly working for the prime contractor and service providers that specialise in aeroacoustics, structures and aerodynamics.

Figure 1: Aerospace application scenario
4.3 Automotive

Within the automotive application activity the architectural vision is to start with tightly coupled propriety systems and progress to a loosely coupled web services Grid architecture based on open standards. This should be done to move from application centric (MSC NASTRAN / ESI PAMCrash) to problem centric analysis services (crash/meshing/assembly). Therefore there is a need to switch from isolated discipline specific databases (CAE/CAT) to transparent secure inter-organisation data access and integration.

Based on the two main stakeholders in this application activity – AUDI/SEAT on one hand and RENAULT on the other hand – there are two basic initial scenarios. The group centred around AUDI is interested in enabling intra-organisation multi-disciplinary simulation (CAE/CAT; crash/NVH) based on MSC.SimManager and MSC NASTRAN. The group centred around Renault is looking into improving the interaction between manufacturer and supplier to evolve a collaborative CAE simulation outsourcing scenario based on ESI PAMCrash.

Regarding the software environments at the end of the project, i.e. after 48 months, the following is planned:

Managing distributed simulation data is a key component of SIMDAT. Within the SIMDAT environment, there is not only data to be consumed and disseminated, but also the analysis services produce a substantial amount of data, which has to be persistent in SIMDAT. As part of persisting the data, its full pedigree needs to be stored, for example in meta databases. The foundation of the project is the assumption that AUDI will use individual implementations at various engineering sites in a coordinated way (meaning with a number of homogeneous assumptions). The implementation will consist in applying information Grid technology to allow analysts in a given location from their MSC.SimManager based workbench (aka CAEBench) to access and act on objects that are stored and initially managed on another location as well as combined objects of the two locations in local engineering actions.

Crash compatibility is a highly involved task. Physical testing of two cars crashing into each other is only possible in special crash test facilities, which allow the simultaneous acceleration of two cars. Such facilities are typically not available at car manufacturers themselves. In addition, there is an increasing demand for performing the so called compatibility crashes at different impact angles, originating from the USA. Using the results of SIMDAT, the goal is to be able to conduct compatibility crash simulations between cars from different car manufacturers over the SIMDAT Grid infrastructure. The Grid security technologies deployed within SIMDAT will allow each car manufacturer to see only the results of his car. The envisioned coupling of CAD, CAE and CAT data will enable the car manufacturer to more quickly identify and resolve any potential design shortcomings discovered in these Grid enabled compatibility crash simulations.

The other automotive application activity Renault/IDEStyle/ESI is concerned with a scenario regarding the interaction between the original equipment manufacturer (Renault) and a supplier (IDEStyle) to evolve a collaborative crash simulation outsourcing scenario based on ESI PAMCrash. The original manufacturer outsources a certain part of the design of a car to a supplier while preserving control and knowledge of the whole vehicle’s design for himself. Therefore only the part to be developed by the supplier and its immediate environment must be known to the supplier while on the other hand remaining secret to the original manufacturer. Work on the model as a whole is given to a trusted third party for calculation.
Results on the outsourced parts are given back only to the supplier while results on the rest of the car are given only to the original manufacturer. Independently from the scenario the manufacturer and the supplier negotiate for the full disclosure of the data afterwards.

The data access prototype will show the interoperability of two simulation data management systems at different locations. Grid technology will be used to enable this. For the 12 month demonstrator it is assumed, that each of the sites for the distributed product development will use MSC.SimManager for the testing and improvement of the functional behaviour of car designs. Grid technology is used to federate MSC.SimManager and provide access to the distributed underlying data bases. A first step into this federation is subject of the demonstrator for the automotive activity.

Access to distributed data bases and distributed data vaults is precondition for the 48 months demonstrator. The 12 months demonstrator will show the comparison of two car crashes whose data is stored at different sites. Furthermore there is a need to have the possibility to create additional post-processing objects (PPOs) on both sides for deeper investigation of the car crashes. On every side the car projects of the other side should “feel” like the local car projects in the navigation frame of MSC.SimManager.

In the design phase there is the opportunity to visit various approaches to solve the distributed simulation data management challenge. From a pure web services based external information broker agent to a middleware provided federated database solution, all will be challenged and individually evaluated to identify possibilities and dependencies brought to the project. Finally, after considering key features and probable necessary adaptations of MSC.SimManager attached to each alternative, the best solution will be chosen.

For this demonstrator a comparison report with data on different sites is to be generated. The demonstrator will use the hardware and software environment, which will be set up by MSC for the Grid infrastructure demonstrator. For this purpose AUDI has generated two geometric variants of the SAMD car and will perform a number of crash simulations and a compatibility crash between the two models. The data access demonstrator is performed using crash simulations on the SAMD car version 2 (coupe) and version 3 (cabriolet) which Audi provides. Model data will be made available on the two reference installations of MSC.SimManager at MSC. Grid technology will be used to fetch the crash evaluation data from the different reference installations.

The second demonstrator is consistent with the long term project goal. Initially only a light demonstrator will be set up. This demonstrator will then evolve in requirements and functionality. The OEM (Renault) uploads data (requirements, CAD, meshes, material law…) for the supplier (IDEStyle). IDEStyle downloads Renault data. IDEStyle does the job with the data (pre processing of PAMCRASH model, calculation, post processing). Renault follows up the tasks and consults the draft deliverables of IDEStyle during virtual project meetings (meshes, PAMCRASH model, analysis). After validation by IDEStyle and Renault, data is transferred to Renault.

The Grid infrastructure needs to have a clearly defined interface to analysis services. Batch as well as interactive analysis services will be run on the system. Services for resource management and job scheduling are mandatory.

For distributed data repositories access and integration a robust and efficient data transport to and from analysis services, including large data volumes (average about two Gbytes per
simulation, six Tbytes per year) must be present. It must be possible to separate metadata and data. A standardisation and federation at conceptual level (door, dashboard, etc) is needed. Very important for the end user is the audit trail preservation.

From a security and privacy point of view access control for data and services, secure data exchange between collaborating organisations, and IPR protection for component suppliers in collaborative crash simulation is mandatory.

Initially the automotive application scenarios require a pragmatic approach. Thereby the delivery of the 12 month prototypes is ensured. Grid infrastructure needed and distributed data repository access software should by and large be available today with only small changes called for. There is a need to start prototyping as soon as possible.

GRIA provides a good starting point. There is support for batch integration of file compute analysis services as well as trust relationships for OEM/Supplier collaborations. The Grid software is based on WS-I standards and integrates fairly easy with OGSA-DAI.

OGSA-DAI provides a good starting point. OGSA-DAI WS-I will be used in the project. Thereby the efficient access to large data repositories is enabled. OGSA-DAI supports distributed ‘same schema’ queries for CAE/CAT integration using minimum common data set.

Consortium partners will provide support and intellectual engagement to partners within the project for both GRIA and OGSA-DAI.
4.4 Meteorology

In 2003 the World Meteorological Organization (WMO) approved the concept of Future WMO Information System (FWIS). The FWIS will provide a single coordinated global infrastructure for the collection and sharing of information in support of all WMO and related international programmes.

WMO has defined a virtual structure for the FWIS, which contains three main actors:
- National Centres (NC)
- Global Information System Centres (GISC)
- Data Collection and Production Centres (DCPC)

As a first step towards the establishment of FWIS, the national weather services of France, Germany and the United Kingdom have volunteered to jointly implement a Virtual GISC (V-GISC). The three V-GISC partners form a cluster and enjoy equal rights and mutually support one another. The European Centre for Medium-Range Weather Forecast (ECMWF) and the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT) are part of the project as DCPCs.

The V-GISC is a distributed database that will provide users with transparent access to datasets located at Météo-France, DWD, the UK MetOffice, ECMWF and EUMETSAT.

The V-GISC concept is being developed within the meteorology activity of the SIMDAT project.

Some key elements of the project are:
- Improve visibility of and access to data through a comprehensive discovery service based on metadata development,
- Add value to existing datasets by enabling diverse databases to be used as a unique virtual resource,
- Offer a variety of reliable delivery services,
- Provide a global access control policy managed by the partners and integrated into their existing security infrastructure.

A user can use the V-GISC according to one of the five global use cases:
- Access data and metadata
- Provide data and metadata
- Manage VO
- Manage V-GISC infrastructure (data communication infrastructure - DCI)
- Monitor and control the V-GISC

The DCI is the backbone of the V-GISC. It is the software infrastructure developed to provide the V-GISC services. The DCI consists of several nodes hosting metadata and data.

The goal of the meteorology application activity is to generate a meteorology portal that provides access to a virtual meteorology database with supporting VO for access control.

Data reside and are managed by each partner. The three main partners (Météo-France, UK Met Office, DWD) will be closely connected and will be seen as a unique entity offering a collection of datasets to the users. To offer this unified view, the distributed database must be easily interfaced with the actual systems (flat file repository, meteorological database,
relational databases). It should also be enough flexible to easily add a new database containing new datasets. For resilience and performance reasons the metadata will be synchronized between the partners and part of the data (the real-time datasets) is replicated on at least two sites. For example if the DWD site database is down the Météo-France site database or/and the UK Met Office site database must be able to deliver the real-time data to DWD users. The replication is configurable and is managed by each partner (can be activated or deactivated). The distributed database will manipulate two different kinds of datasets:

**Real-time data:** This can be the observation data, model outputs, post-process data, time critical products or warnings. The real-time term is applicable to the data only within 24-48 hours after the data birth date. After that, the data is treated as a non-real time data. These datasets are produced several times within a day and should be distributed within one hour. The average size of daily observations dataset is 58 Megabytes. Currently more and more satellite data is produced and used within the meteorological community and the quantity of daily real-time data is growing rapidly (2 GB produced daily).

The V-GISC will develop performance targets with respect to for example internal reliability and timeliness of data exchange with its neighbours depending on the types of data being exchanged. These targets will be published as part of the operating specifications of the V-GISC.

**Non real-time data:** This is the data contained within the meteorological archive. These data are usually stored on tapes and implies asynchronous retrievals. For example ECMWF runs an archive called MARS. So far 1 Petabyte has been archived and is accessible to ECMWF users. The Data Communication Infrastructure must be able to handle a dataset of few Terabytes but not in a time-critical request.

Metadata are a critical component of the data communication infrastructure. Metadata are required for the discovery, browsing and access. The internal DCPCs will use this infrastructure to update the V-GISC catalogue. The metadata updates will be synchronized among the partners.

The catalogue will be accessible to anybody and a discovery service will be implemented. A query interface will be offered to request sets of data. A subscription service to the datasets will also be implemented. The users will subscribe to different data and will receive it daily when available.

Quality of service mechanisms will be implemented. The cost of a request will be estimated in term of resources necessary to offer the service. The request will be then placed in a queue and the position in the queue will depend on parameter such as the cost of the request, the user’s priority, …. Prioritization mechanisms will be implemented in order to deliver data, such as warning messages, as soon as they are received by the V-GISC.

The data communication infrastructure DCI has to be built to federate all the partners’ data repositories. Among the main challenges that have to be solved in order to build the DCI is the implementation of a virtual database providing the following services:

- Create a unified view of all the shared datasets through a distributed catalogue.
- Define a metadata format containing information to locate and identify the data, to describe the data access policy and to describe the available meteorological data for discovery.
- Maintain the distributed catalogue amongst the partners using synchronization mechanisms
- Give access to the legacy meteorological databases
- Implement data replication and cache mechanisms
- Preserve the data integrity

Another challenge is the implementation of data access services:
- Collection and dissemination services that support various efficient and reliable transport mechanisms
- Quality of service (QoS): traffic prioritization, queuing mechanisms
- Discovery service by browsing a hierarchical catalogue or using a keyword search engine
- Interactive interface authorizing humans to easily access the data
- Batch interface authorizing programs to easily access the data
4.5 Pharmaceuticals
4.5.1 Overview

In the last decades, the advances in the life science sector have facilitated the rapid acquisition of vast amounts of data e.g. in the diverse genome sequencing projects or in high throughput screening of compounds against drug targets. Academic and industrial researchers in the life sciences community use this data for various experiments. These experiments allow the scientist to investigate or verify a hypothesis that they may have about a particular problem or domain. Such in-silico experiments are, by their very nature, hypothesis driven, ad-hoc and highly specialised to the particular problem they are associated with. For example, in medicine, sequences provide a basis for the study of susceptibility to disease and the development of new preventative and therapeutic approaches whereas, in cell biology, the interactions between components of cellular circuitry can be studied. The pharmaceuticals activity will deploy and use Grid technology to provide added value to existing data integration technology in supporting collaborative bioinformatics experiments.

Life science research is supported by a collaboration of research institutions called EMBNet that provide national scientific communities throughout the world with access to high performance computing resources, specialised databases and up-to-date software. Each research institution within EMBNet is known as an EMBNode and is responsible for maintaining a set PSE’s, analysis tools and bioinformatics databases such as (EMBL, SWISS-PROT, etc). There are approximately 1200 different data providers and each EMBNode maintains a subset of the overall data. New data is published to the community when researchers report their results through academic papers. It is a precondition for paper publication that the bioinformatics data is available in the public domain. Researchers can access EMBNet resources by providing a nominal yearly fee that gives access to all data and analysis services along with a disk quota that can be extended on request.

In industry, researchers also use public data providers but augment this information with proprietary data generated within their organisation. Pharmaceutical companies do not typically access EMBNet directly but maintain in-house databases due to confidentiality constraints. Even the knowledge of the types of queries being performed is commercially sensitive information as it gives competitors information about current drug targets.

The cost of distributing and maintaining databases produced by public data providers is a significant problem for both EMBNodes and pharmaceutical companies. Bioinformatics data is generated at an incredible rate and databases can be updated on a daily basis. Up-to-date data is important to researchers, as additional sequence data can significantly change the results of some analysis. Organisations typically schedule database updates according to their business needs, for example, daily or bi-weekly. The maintenance of databases requires organisations to manually monitor data providers for new database releases and acquire the release either by direct download or CD. Updates can be computationally expensive, for example, updating an EMBL database (>400G Bytes) within a SRS server can take days to calculate the necessary indexes (obviously depending upon the target platform).

Data providers distribute data in a variety of standard (XML, ASN.1) and proprietary data formats (FASTA, GenBank, SwissProt). Researchers execute cross-database queries using tools like SRS that provides integration of these diverse and complex data structures. At present, to do a cross-database query SRS requires all data and indexes to be co-located.

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20 In silico experiments are procedures using computer based information repositories and computational analysis adopted for testing hypotheses or to demonstrate known facts.
pharmaceutical activity is looking to federate SRS so that distributed cross-database queries can be supported reducing the need to support an entire set of databases at a single server.

Researchers use a wide variety of domain specific PSE’s and analysis tools to support their experiments such as SRS for cross-database sequence similarity searching. Some analysis tools such as those adopting brute force algorithms can be computationally expensive lasting many hours. Researchers traditionally chain together database searches and analytical tools, using complex scripts to overcome incompatibilities in data formats, or by manually cutting and pasting between web interfaces. These in silico experiments are usually undertaken without support for the scientific process of managing, sharing and reusing the results, their provenance, and the methods used to generate them. Management of the scientific process is important should the data be judged erroneous at a later date. The researcher can then determine the results that need to be ignored or experiments that should be rescheduled. Currently, there are no standards for database description metadata and versioning information. Each data provider adopts its own approach with some providers’ not even publishing version information; these have to be derived from the date of download. For multiple distributed SRS servers containing replica databases it is important that database versions are synchronized. The database lifecycle is currently managed manually or by a technology called PRISMA.

The pharmaceuticals activity is looking to develop new business models for carrying out bioinformatics research that will enable collaborative experiments within the commercial and academic communities that supports a managed scientific process. These business models are in the early stages of development and will be further defined during the development of the first demonstrator. An example possible business model could be based on a project team assembled by a pharmaceutical company for the development of a new drug. The team could consist of a set of trusted data providers and analysis service providers along specialist scientific teams with the company. There may be situations when smaller organisations could provide specific areas of expertise in the development process and could join the virtual organisation. Researchers define in silico experiments that execute workflows querying data sources and executing analysis services. When a researcher executes a workflow the infrastructure manages generated data and derived knowledge along with provenance about the experiment allowing other scientists to interpret the experiments context. As the scientists perform experiments results are generated that should shared with authorised team members. Periodically, when results are seen to provide value beyond the project team they are validated and published the wider community either within a proprietary company database or public database.